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THE EFFECT OF THE SURFACE ON THE MAGNETIC PROPERTIES OF AN ELECTRON GAS

By

Harvey Brooks and F. S. Ham

March 10, 1953

Technical Report No. 169

Cruft Laboratory
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TR169

The Effect of the Surface on the Magnetic Properties of an Electron Gas

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I.

Introduction

A number of papers[1-13] have been published in the last twenty years concerning the determination of the magnetic susceptibility of a system of free electrons or of electrons confined to a box, and a variety of elegant methods have been applied. It has not been altogether clear, however, to what extent the walls of the system could be neglected in some of these calculations, and the dependence of the susceptibility on the form of the wall potential has not been adequately investigated. Since in fact the walls play an essential role, a derivation which explicitly considered them seemed desirable. The authors believe that the present treatment offers a clear picture of the physical situation, some worth-while criticisms of results obtained by other methods, and a few useful modifications of the mathematical methods previously used.

It is well known[14,15] that in classical physics the positive moment contributed by electrons that collide with the walls of the system exactly cancels the negative moment of electrons far from the walls. Van Vleck[5] and Teller[6] showed that a similar balancing occurs in quantum mechanics (with a non-zero resultant)

and gave arguments to justify the value for the magnetic susceptibility obtained by Landau[9] from the free energy. However, Teller's argument was for an infinite plane wall, and Van Vleck's required the use of the old quantum mechanics, and it is not clear to what extent either justifies the more recent calculations by Landau[1] and others of the oscillatory De Haas-Van Alphen terms. We shall first give an improved argument for a cylindrical box which makes clear this balancing of diamagnetic and paramagnetic states and determines with the WKB approximation the nature of the boundary states. We shall then give a more detailed derivation needed to establish corrections to the terms in the susceptibility that dominate at high field strengths. This will show that the usual treatments[1] give the De Haas-Van Alphen terms correctly for "strong fields" and that the only important correction to the Landau steady diamagnetism is a term of the form of the "surface diamagnetism" recently reported by Osborne[7] and Steele[8]. Unfortunately, the magnitude and sign of both this surface correction and the susceptibility of intermediate and small systems obtained by Dingle's method[3,4] depend rather sensitively on the assumptions made about the form of the wall potential. This result throws some doubt on the accuracy of the WKB method in such calculations. The following derivation is valid only if the radius R of the confining box is considerably larger than the classical orbit radius $R_c = \frac{c}{eH}\sqrt{2m\zeta}$ of an electron moving in a plane perpendicular to the magnetic field with energy equal to the Fermi energy ζ of the system--the "strong field" case. Finally we shall give heretofore unpublished results for the model proposed by Darwin[10] to show some fundamental differences from the usual electron-in-a-box model.

II.

Methods of Calculating the Magnetic Moment

The usual procedure has been to calculate the magnetic moment M from the Helmholtz free energy F by the formula

$$M = -\left(\frac{\partial F}{\partial H}\right)_{T,V,N} \tag{2.1}$$

It is, however, evident that if the electrons are independent except in so far as they obey the exclusion principle when Fermi statistics are used, then the moment of the system should also be given by the sum of the moments of the individual electron states weighted with the probability that the state is occupied.[5,7] Thus with Fermi statistics we should have

$$M = \sum_i \left(-\frac{\partial \varepsilon_i(H)}{\partial H}\right) \frac{1}{1+e^{(\varepsilon_i(H)-\zeta)/kT}}, \tag{2.2}$$

where ζ is determined by the condition

$$N = \sum_i \frac{1}{1+e^{(\varepsilon_i(H)-\zeta)/kT}}, \tag{2.3}$$

N being the total number of electrons in the system, and the sum being taken over all single electron states. On the other hand, the free energy is given by

$$F = N\zeta - kT \sum_i \ln[1+e^{(\zeta-\varepsilon_i(H))/kT}], \tag{2.4}$$

and since by (2.3) $\frac{\partial F}{\partial \zeta} = 0$, (2.1) and (2.2) give the same result provided the limits of summation in (2.4) and the degeneracy of states with a common energy (if we should use the index i to label a collection of states with the same energy instead of a single state) do not depend on H.

However, for a system confined by a cylindrical box of cross section A with its axis parallel to the uniform magnetic field, the energies of states unperturbed by the walls are[16]

$$\varepsilon_{nk_z} = \frac{\hbar^2 k_z^2}{2m} + (2n+1)\beta H, \qquad n = 0,1,2,\ldots. \tag{2.5}$$

where $\beta = \frac{e\hbar}{2mc}$, k_z is the component of the propagation vector along the axis, and the degeneracy of each such (n,k_z) level is to first approximation[3,8] $\frac{eHA}{hc}$, neglecting spin degeneracy. As remarked by Van Vleck[5] and Osborne,[7] if we use only these energy states (2.5) and this degeneracy in (2.2), we find a large negative total moment of magnitude greater than $N\beta$, whereas (2.4) and (2.1) yield the usual Landau result (for $(\beta H << \zeta)$),

$$M = -\frac{4m\beta^2 V}{h^2}\left(\frac{N\pi^2}{9V}\right)^{1/3} H = -\frac{N\beta^2 H}{2\zeta} = -\frac{n(\zeta)\beta^2 H}{3}, \qquad (2.6)$$

plus the periodic De Haas-Van Alphen terms. Here $n(\zeta)$ is the density of states (including spin degeneracy) in the energy scale at the Fermi level ζ, and the second expression shows (2.6) to be much less in magnitude than $N\beta$. Our first problem is, then, to show that the difference between these methods is removed when we include the positive moments of the boundary states in our summation (2.2).

III.

The Boundary States in the WKB Approximation

We consider the Schrödinger equation satisfied by the wave function of a single electron state in a cylindrical box of length L and radius R with its axis parallel to the uniform magnetic field, in which we neglect all interaction between electrons:

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\right]\psi - i\beta H\frac{\partial\psi}{\partial\phi} + \frac{e^2H^2}{8mc^2}(x^2+y^2)\psi = E\psi \qquad (3.1)$$

for $r < R$, and the boundary condition $\psi(R) = 0$. On separating in cylindrical coordinates, we put

$$\epsilon' = E - \frac{\hbar^2 k_z^2}{2m} - \beta H s$$

$$\psi = e^{ik_z z}\, e^{is\phi} f(r), \qquad (3.2)$$

$$s = 0, \pm 1, \pm 2, \ldots,$$

and get as the equation for f(r)

$$-\frac{\hbar^2}{2mr}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)f(r) + \left[\frac{\hbar^2 s^2}{2mr^2} + \frac{e^2H^2r^2}{8mc^2}\right]f(r) = \varepsilon' f(r). \quad (3.3)$$

We now make the substitution $r = e^x$, $f(r) = g(x)$, which puts (3.3) in a form suitable for the WKB approximation:

$$\frac{\partial^2 g(x)}{\partial x^2} + \frac{2m}{\hbar^2}\left[\varepsilon' e^{2x} - \frac{\hbar^2 s^2}{2m} - \frac{e^2H^2}{8mc^2}e^{4x}\right]g(x) = 0. \quad (3.4)$$

This determines ε' in terms of s and n through the phase integral condition (after transformation back to r)

$$\int_{r_1}^{r_2}\left[2m\left(\varepsilon' - \frac{\hbar^2 s^2}{2mr^2} - \frac{e^2H^2r^2}{8mc^2}\right)\right]^{\frac{1}{2}} dr = (n + \tfrac{1}{2})\hbar\pi, \quad (3.5)$$

where r_1 and r_2 are the two positive zeros of the quantity under the square root, provided thar $r_2 \leq R$. This condition yields

$$\varepsilon' = (2n + |s| + 1)\,\beta H, \quad (3.6)$$

and the energies are given by (2.5). If, however, $r_1 < R < r_2$, then the upper limit of integration is R, and it is evident that for given n and s, ε' will be increased over the value (3.6).[17] We note that the quantum numbers n, s, and k_z and the spin orientation completely specify a single state, which according to the exclusion principle can be occupied by no more than one electron.

The integral in (3.5) with R as the upper limit can be evaluated exactly,[18] but the result is a complicated implicit equation for ε' which can be solved only with great difficulty. Fortunately, when s is large, the effective radial "potential" in (3.3),

$$v(r) = \frac{\hbar^2 s^2}{2mr^2} + \frac{e^2H^2r^2}{8mc^2} \quad (3.7)$$

has a sharp minimum at

$$r_o = \sqrt{\frac{2\hbar|s|c}{eH}} \quad (3.8)$$

and to excellent accuracy may be approximated by the first terms of a power series,

$$v(r) \cong \beta H|s| + \frac{e^2H^2}{2mc^2}(r-r_o)^2. \qquad (3.9)$$

Higher terms in the series may be neglected for energies of the order of ζ provided $R >> R_c$, the condition mentioned in the introduction. For the present we consider only states with non-positive values of s, so that we have from (3.2), (3.5), and (3.9), using $\varepsilon = \varepsilon' - \beta H|s| = E - (\hbar^2 k_z^2)/2m$

$$\int_{r_1}^{r_2}\left[2m\left(\varepsilon - \frac{e^2H^2}{2mc^2}\right)(r-r_o)^2\right]^{\frac{1}{2}} dr = (n + \tfrac{1}{2})\hbar\,\pi. \qquad (3.10)$$

Setting $\varepsilon = (2n+1)\beta H$, we find that the range of r for which the quantity under the square root is positive is

$$\Delta r = 2r_o \sqrt{\frac{(n+\frac{1}{2})}{|s|}}\ , \qquad (3.11)$$

so that the wave functions of the vast majority of occupied states are highly localized radially at a distance r_o from the axis of the box, provided only that

$$|s|_o = \frac{eHR^2}{2\hbar c} = \frac{eHA}{hc}\quad , \qquad (3.12)$$

the number of states with common spin orientation and common n and k_z and $r_o \leq R$, is very much greater than $\zeta/2\beta H \sim n+\frac{1}{2}$. This is in particular true for boundary states, for which $r_o \sim R$. The quantity Δr in (3.11) is actually the diameter $\frac{2c}{eH}\sqrt{2m\varepsilon}$ of the orbit of a classical electron with "transverse energy" ε.

We determine ε as a function of (r_o-R) by solving (3.10) with R replacing r_2 as the upper limit of integration. On defining

$$y = \frac{\varepsilon}{\beta H}\quad , \quad x = (r_o-R)\left(\frac{eH}{\hbar c}\right)^{\frac{1}{2}}\ , \qquad (3.13)$$

we are led to the system of equations

$$y = \frac{x^2}{z^2} = \frac{(2n+1)\pi}{\cos^{-1}z - z(1-z^2)^{\frac{1}{2}}} = (2n+1)g(z) ,$$
$$x = \frac{z(2n+1)^{\frac{1}{2}}\sqrt{\pi}}{(\cos^{-1}z-z(1-z^2)^{\frac{1}{2}})^{\frac{1}{2}}} = (2n+1)^{\frac{1}{2}}f(z), \tag{3.14}$$

where z is a parameter with the range $-1 \leq z \leq 1$. These have been solved numerically for n = 0,1,2, and the results are plotted in Fig. I.

The moment of a state of given n and s is given by

$$M_{n,s} = -\left(\frac{\partial\varepsilon_{n,s}}{\partial H}\right)_s = -\left[\left(\frac{\partial\varepsilon_{n,s}}{\partial H}\right)_{r_o} + \left(\frac{\partial\varepsilon_{n,s}}{\partial r_o}\right)_H \frac{dr_o}{dH}\right]. \tag{3.15}$$

For "bulk states" far from the wall, we have from (3.10), as usual, $\varepsilon_{n,s} = (2n+1)\beta H$ and $M_{n,s} = -(2n+1)\beta$, but for boundary states given by (3.14) it is readily seen that the first term in (3.15) is negligible compared with the second. The moment is therefore positive, since $(\partial\varepsilon/\partial r_o)_H > 0$ and from (3.8)

$$\frac{dr_o}{dH} = -\frac{1}{H^{3/2}}\left(\frac{\hbar|s|c}{2e}\right)^{\frac{1}{2}}. \tag{3.16}$$

Together with (3.13) and (3.14), this yields for boundary states

$$\frac{M_{n,s}}{\beta} = \frac{1}{\sqrt{2}}\frac{\partial y}{\partial x}\sqrt{|s|_o} = \frac{(2n+1)^{\frac{1}{2}}(2\pi|s|_o)^{\frac{1}{2}}(1-z^2)^{\frac{1}{2}}}{\cos^{-1}z(\cos^{-1}z-z(1-z^2)^{\frac{1}{2}})^{\frac{1}{2}}}, \tag{3.17}$$

which is plotted in Fig. II for n = 0,1,2. We note that the moment of a single boundary state is proportional to the square root of the degeneracy $|s|_o$ given in (3.12). As we shall see from (4.2), (3.11), and (3.8), the number of occupied states is proportional to the same quantity, so that the total moment contributed by boundary electrons is proportional to $|s|_o$.

IV.

Approximate Calculation of the Total Moment

We consider first the system discussed by Peierls,[11] with N electrons in a "two-dimensional" system with common value of k_z and common spin orientation, at the absolute zero of temperature. For very strong magnetic fields the degeneracy $\frac{eHA}{hc} = |s|_0$ of the n = 0 level is larger than N, so that all electrons are in the lowest bulk state, and the moment of the system is $-N\beta$. As H is lowered, the r_0 of each state increases by (3.8) until some occupied states are forced up into the "tail" of Fig. I. We shall calculate the moment of this tail at the field strength at which the uppermost filled state in the tail is just level with the n = 1 bulk states, so that for a further decrease in H electrons must "overflow" from the n = 0 tail to n = 1 bulk states, if the system is to remain in thermal equilibrium. Then from (3.15), neglecting $(\frac{\partial\varepsilon}{\partial H})_{r_0}$, we have

$$M_{tail} = \int_{\text{filled tail}} dr_0 \rho(r_0)\left(-\left(\frac{\partial\varepsilon}{\partial r_0}\right)_H \frac{dr_0}{dH}\right), \tag{4.1}$$

where $\rho(r_0)$ is the density of n = 0 states in terms of the parameter r_0 and, since n and s completely specify a state, is given from (3.8) by

$$\rho(r_0) = (\frac{2eH\ |s|}{\hbar c})^{\frac{1}{2}}. \tag{4.2}$$

From this and (3.16), together with the observation that for a large system the spread in $|s|$ of the states in the occupied part of the tail is negligible compared with the value of $|s|_0$ itself, we see that we can take $|s|_0$ from under the integral, getting

$$M_{tail} = \frac{|s|_0}{H} \int_{\text{filled tail}} dr_0 (\frac{\partial\varepsilon}{\partial r_0})_H = \frac{|s|_0}{H} [\varepsilon]_{bottom}^{top}. \tag{4.3}$$

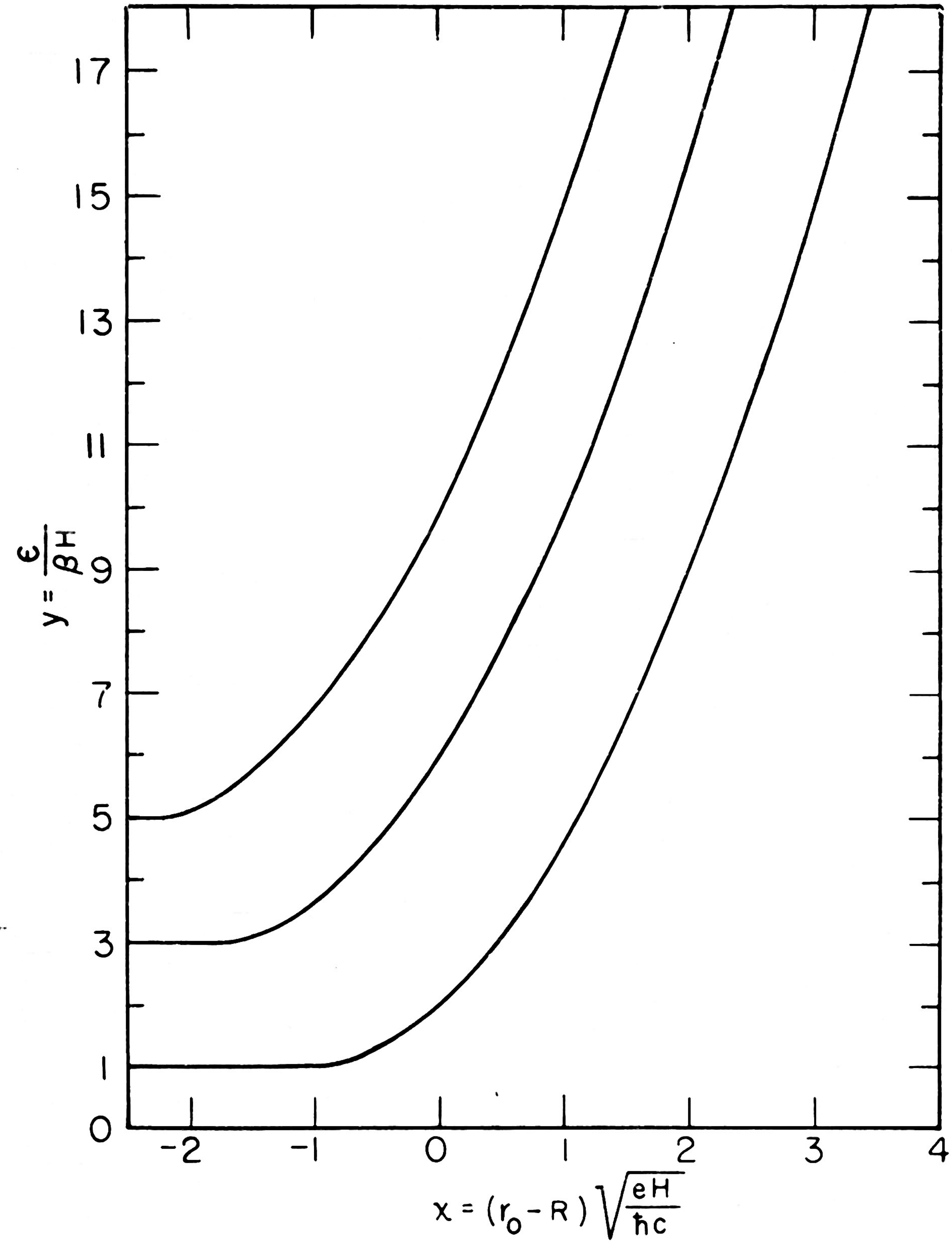

FIG. I ENERGY OF THE BOUNDARY STATES. THE QUANTITIES x AND y ARE DEFINED IN (3.13)

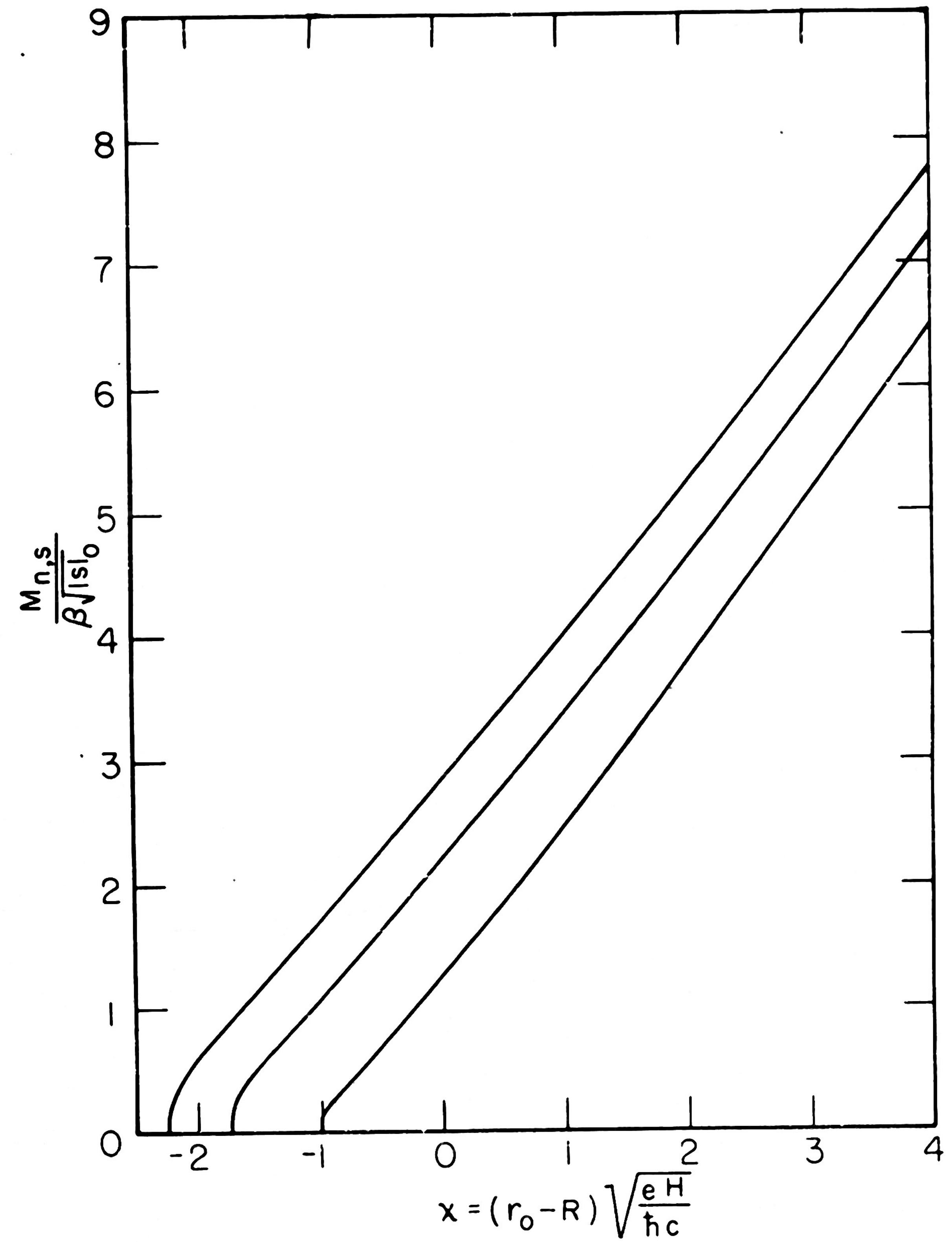

FIG. II MOMENT OF THE BOUNDARY STATES

Since the filled part of the tail stretches between the unperturbed bulk states n = 0,1, we have finally

$$M_{tail} = \frac{|s|_o}{H} 2\beta H = 2N\beta . \tag{4.4}$$

Hence on adding to this the moment of all the n = 0 bulk states, whose number is not appreciably diminished from N by the loss of a few states to the tail, we see that the total moment is $N\beta$, as given by Peierls. Continuing this argument as the higher bulk levels fill up, we find the same oscillation between $-N\beta$ and $N\beta$ found by Peierls. We note, however, that the change from $-N\beta$ to $N\beta$ is very rapid but not discontinuous and in fact occurs over a range $\Delta H/H \sim 2/\sqrt{|s|_o}$.

It is now a simple matter to consider finite temperature and to justify (2.1) and (2.4) from (2.2). The moment contributed by the bulk states is as usual (for given spin orientation)

$$M_{bulk} = -\frac{eHA}{hc}\sum_{n=o}^{\infty}(2n+1)\beta\frac{L}{2\pi}\int_{\infty}^{\infty}dk_z\frac{1}{1+e^{\left[(2n+1)\beta H+\frac{\hbar^2k_z^2}{2m}-\zeta\right]/kT}}, \tag{4.5}$$

whereas the moment contributed by electrons in the tails is

$$M_{tails} = -\frac{L}{2\pi}\sum_{n=o}^{\infty}\int_{\infty}^{\infty}dk_z\int_{tail\ n}dr_o\rho(r_o)\left(\left(\frac{\partial\varepsilon}{\partial r_o}\right)_H\frac{dr_o}{dH}\right)\cdot\frac{1}{1+e^{\left[\varepsilon(n,r_o,H)+\frac{\hbar^2k_z^2}{2m}-\zeta\right]/kT}} \tag{4.6}$$

Again using (3.16) and (4.2), taking $|s|_o$ out of the integral on assuming its spread negligible over the part of the tail for which $\frac{1}{1+e^{\left[\varepsilon+\frac{\hbar^2k_z^2}{2m}-\zeta\right]/kT}}$ is appreciable, and using (3.12), we have

$$M_{tails} = -\frac{kTAeL}{2\pi\hbar c}\sum_{n=o}^{\infty}\int_{-\infty}^{\infty} dk_z \int_{tail\ n} dr_o \frac{\partial}{\partial r_o}$$

$$\cdot \left[\ln\left(1+e^{[\zeta-\varepsilon(n,r_o,H)-\frac{\hbar^2 k_z^2}{2m}]/kT}\right) \right] \quad (4.7)$$

On carrying out the integration over the tails, which extend from the energies of the unperturbed n levels to infinity, we get

$$M_{tails} = \frac{kTeAL}{2\pi\hbar c}\sum_{n=o}^{\infty}\int_{-\infty}^{\infty} dk_z \ \ln\left(1+e^{[\zeta-(2n+1)\beta H-\frac{\hbar^2 k_z^2}{2m}]/kT}\right) . \quad (4.8)$$

Combining this with (4.5) we see that we have for the total moment

$$M = -\frac{\partial}{\partial H}\left\{-\frac{kTAeHL}{2\pi\hbar c}\sum_{n=o}^{\infty}\int_{-\infty}^{\infty} dk_z \ \ln\left(1+e^{[\zeta-(2n+1)\beta H-\frac{\hbar^2 k_z^2}{2m}]/kT}\right)\right\} \quad (4.9)$$

where we treat ζ as a constant parameter in the differentiation. This is exactly the formula obtained from (2.1) and (2.4) when we form F using only the energies of the bulk states and the degeneracy (3.12), provided we use (2.3) to eliminate terms involving $\frac{d\zeta}{dH}$, and neglect states of positive s. Hence to the extent that s has negligible spread over the occupied portions of the tails, the usual formula (2.1) is valid despite the field-dependent degeneracy. We now recognize the vital role played by the boundary states in cancelling a large part of the bulk diamagnetism, and we can no longer suppose such calculations applicable to electrons that are completely free.

Had we used Boltzmann statistics instead of Fermi statistics, the arguments would have gone through similarly, and, in fact, if we change our parameter of integration in the expression analogous to (4.7) from r_o to s, we get essentially the boundary term in equation (68) of Van Vleck's derivation.[5]

V.

Correction Terms in the Total Moment

Instead of trying to refine the above argument directly in order to obtain correction terms when the spread in s is appreciable, we now turn to a more elegant derivation which is more easily handled but which shows the nature of the balancing of bulk diamagnetism and surface paramagnetism less clearly than the above. We consider the system of Section III with the cylindrically symmetric radial potential generalized to an arbitrary $V(r)$ so that in the Schrödinger equation (3.1) $E\psi$ is replaced by $(E-V(r))\psi$. The separation of variables used in (3.2) is still valid, and we now define r_o by (3.8). Temporarily we restrict attention to non-positive values of s and require that the "transverse energy" parameter $\varepsilon = E - (\hbar^2 k_z^2/2m)$ vary sufficientlyslowly as a function of $|s|$ to allow us to replace sums over $|s|$ occurring in expressions for the moment and free energy by integrals over $|s|$. This is equivalent to the requirement that our fields be strong, that is, that $R >> R_c$. We require also that the length L of the cylinder parallel to the field be long enough so that sums over the allowed values of k_z may be replaced by integrals over k_z with the density $L/2\pi$. We have then for the total moment of electrons with a common spin orientation[19]

$$M = -\frac{L}{2\pi}\int_{-\infty}^{\infty} dk_z \sum_{n=o}^{\infty}\int_0^{\infty} d|s| \left(\frac{\partial\varepsilon}{\partial H}\right)_{|s|} \frac{1}{1+e^{(\varepsilon+\frac{\hbar^2 k_z^2}{2m}-\zeta)/kT}} . \qquad (5.1)$$

Integrating by parts in $|s|$, noticing that contributions from the limits of integration vanish, taking the derivative with respect to H (regarding ζ as a constant parameter) from under the integral signs on the reasonable assumption that $\partial^2\varepsilon/\partial H\partial s = \partial^2\varepsilon/\partial s\partial H$, and finally changing our parameter of integration from $|s|$ to r_o by (3.8), we have

$$M = -\frac{\partial}{\partial H}\left\{\frac{L}{2\pi}\frac{kTeH}{2\hbar c}\int_{-\infty}^{\infty} dk_z \sum_{n=0}^{\infty}\int_0^{\infty} r_o^2\, dr_o \frac{\partial}{\partial r_o}\ln\left(1+e^{(\zeta-\varepsilon(n,r_o,H)-\frac{\hbar^2 k_z^2}{2m}/kT}\right)\right\} \tag{5.2}$$

The bracketed quantity is, of course, the quantity $(F-N\zeta)$ (still neglecting states with s positive). We may also derive (5.2) from (5.1) by first changing our parameter of integration to r_o, using (3.15), and then performing the necessary integration by parts. We shall now consider the evaluation of $(F-N\zeta)$ in the form appearing in (5.2).

We first set $E = \varepsilon + \frac{\hbar^2 k_z^2}{2m}$, change from k_z to E as a parameter of integration, and integrate by parts in E, obtaining

$$F-N\zeta = \frac{L}{2\pi}\frac{eH}{\hbar c}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}\int_0^{\infty}\frac{\partial f_o}{\partial E}\,dE\sum_{n=0}^{\infty}\int_0^{\delta(n,H,E)} r_o^2\left(\frac{\partial\varepsilon(n,H,r_o)}{\partial r_o}\right)(E-\varepsilon)^{\frac{1}{2}}\,dr_o, \tag{5.3}$$

where f_o is the Fermi function $\frac{1}{1+e^{(E-\zeta)/kT}}$ and $\delta(n,H,E)$ is that value of r_o for which $\varepsilon = E$. We may replace $\delta(n,H,E)$ by ∞ if we consider $(E-\varepsilon)^y$ to be identically zero whenever $\varepsilon > E$, as we shall do henceforth.

We now specialize $V(r)$ to be constant over our system except for a rapid rise at the wall. Then only for states in the tail will ε depend on r_o, and we may replace zero in (5.3) as the lower limit of integration over r_o by $(R-\Delta r_{on})$, the value of r_o at which the n^{th} tail starts to rise.[20,21] The tail rises rapidly in energy so that r_o^2 differs only slightly from R^2 for occupied states in the tail, and we may advantageously use the expansion

$$r_o^2 = R^2 + 2R(r_o-R) + (r_o-R)^2. \tag{5.4}$$

When we use the first term, R^2, in (5.3), the integral over r_o is immediately and exactly integrable. The only contribution comes from the lower limit of integration, where the energy levels are those of the free electron, $(2n+1)\beta H$. This is the value for the free energy derived by Landau,[1] Sondheimer and Wilson,[2] and Dingle.[3]

We see that the evaluation of this term in the expansion is exact, independently of any approximations that must be made in determining ε in the energy tail.

The evaluation of the contribution to F of the second and third terms in (5.4) will depend on our approximations in determining ε. In the following work we shall assume the V(r) of Section III, an infinite potential jump at the wall, and use the approximate results of (3.13) and (3.14). From these equations we see that to the accuracy of our use of the WKB method and the approximate potential (3.9), the n^{th} tail starts up at $\Delta r_{on} = \left(\frac{\hbar c}{eH}(2n+1)\right)^{\frac{1}{2}}$, that $(r_o - R) = \left(\frac{\hbar c}{eH}(2n+1)\right)^{\frac{1}{2}} f(z)$, and that $\varepsilon = (2n+1)\beta H\, g(z)$. Hence it is convenient to change our variable of integration in (5.3) from r_o to z, which together with (5.4) gives us

$$F - N\zeta = \frac{L}{2\pi}\frac{eH}{\hbar c}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int_0^\infty \frac{\partial f_o}{\partial E}\, dE \sum_{n=o}^{\infty} \int_{-1}^{1} dz \left\{ R^2 + 2R\left(\frac{2\hbar c}{eH}(n+\tfrac{1}{2})\right)^{\frac{1}{2}} f(z) \right. \tag{5.5}$$

$$\left. + \frac{2\hbar c}{eH}(n+\tfrac{1}{2})(f(z))^2 \right\} 2\beta H(n+\tfrac{1}{2}) \frac{dg(z)}{dz} \left(E - 2\beta H(n+\tfrac{1}{2})g(z)\right)^{\frac{1}{2}}.$$

We shall now consider separately each of the three terms, which we call $(F-N\zeta)_o \sim R^2$, $(F-N\zeta)_1 \sim R$, and $(F-N\zeta)_2 \sim 1$, and in each we shall reverse the order of integration over z and summation over n. We see that we have to consider sums of the form

$$\sum_{n=o}^{\infty} (n+\tfrac{1}{2})^x \left(E - 2\beta H\,(n+\tfrac{1}{2})g(z)\right)^y , \tag{5.6}$$

where, as already remarked, we consider the second factor identically zero when $2\beta H(n+\frac{1}{2})g(z) > E$. We now use the Poisson sum formula[3]

$$\sum_{n=o}^{\infty} f(n+\tfrac{1}{2}) = \sum_{r=-\infty}^{\infty} (-1)^r \int_o^\infty e^{2\pi i n r} f(n)\, dn, \tag{5.7}$$

according to which (5.6) equals

$$\sum_{r=-\infty}^{\infty} (-1)^r (\xi)^{x+1} E^y \int_0^1 e^{2\pi i \xi r u} \cdot u^x (1-u)^y du, \tag{5.8}$$

where we have put $\xi = \frac{E}{2\beta H g(z)}$ and $u = n/\xi$.

We must now examine the function

$$V_{xy}(v) = \int_0^1 e^{ivu} u^x (1-u)^y \, du, \tag{5.9}$$

in which we may expand the exponential in its Taylor series and use the beta-function formula,

$$\int_0^1 u^m (1-u)^n du = \frac{\Gamma(n+1)\,\Gamma(m+1)}{\Gamma(n+m+2)} , \tag{5.10}$$

to obtain the expansion

$$V_{xy}(v) = \sum_{s=0}^{\infty} \frac{(iv)^s}{s!} \frac{\Gamma(x+s+1)\,\Gamma(y+1)}{\Gamma(x+y+s+2)} . \tag{5.11}$$

Comparing this with the expansion[22] of the confluent hypergeometric function $M_{k,m}(z)$, we find that

$$V_{xy}(v) = (iv)^{-\frac{1}{2}-m} e^{\frac{iv}{2}} \frac{\Gamma(x+1)\,\Gamma(y+1)}{\Gamma(x+y+2)} M_{k,m}(iv), \tag{5.12}$$

where $k = (y-x)/2$, and $m = (x+y+1)/2$. A useful property is that

$$\frac{dV_{xy}(v)}{dv} = i\, V_{x+1;y}(v) . \tag{5.13}$$

The asymptotic expansion of $V_{xy}(v)$ for $v > 0$ is derived from that of $M_{k,m}(z)$:[23]

$$V_{xy}(v) \sim \Gamma(y+1)e^{iv}\, e^{\frac{-\pi i}{2}(y+1)}\,(v)^{-(y+1)}(1+0(\tfrac{1}{v}))$$

$$+\Gamma(x+1)\, e^{\frac{\pi i}{2}(x+1)}\,(v)^{-(x+1)}\,(1+0(\tfrac{1}{v})). \qquad (5.14)$$

The expansion for $v < 0$ is obtained from this by replacing v by its absolute value and taking the complex conjugate of the formula, since from (5.9), $V_{xy}(-|v|) = V^{*}_{xy}(|v|)$.

Hence (5.8) becomes

$$\sum_{r=-\infty}^{\infty} (-1)^r\, E^{x+y+1}\, \left(\frac{1}{2\beta Hg(z)}\right)^{x+1} V_{xy}\left(\frac{\pi rE}{\beta Hg(z)}\right). \qquad (5.15)$$

To evaluate $(F-N\zeta)_o$, we use the usual procedure on (5.3) in order to avoid any appearance of making an approximation, replace r_o^2 by R^2, integrate over r_o, and then use the Poisson sum. The result is

$$(F-N\zeta)_o = \frac{LR^2}{6\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{\infty} \frac{\partial f_o}{\partial E}\, dE\, E^{5/2} \sum_{r=-\infty}^{\infty} (-1)^r\, V_{c;\frac{3}{2}}\left(\frac{\pi rE}{\beta H}\right). \qquad (5.16)$$

The $r = 0$ term is evaluated using (5.9) and (5.10). The others may be changed in the conventional fashion[1,2] with the formula

$$V_{o;\frac{3}{2}}(v) = \frac{i}{v} - \frac{3i}{2v} V_{o;\frac{1}{2}}(v) = \frac{i}{v} + \frac{3}{2v^2} - \frac{3}{4v^2}\, e^{iv}\, V_{-\frac{1}{2};o}(-v). \qquad (5.17)$$

The series in (5.16) from the first term in (5.17) vanishes if we pair off terms with $r = \pm|r|$. In the series from the second term in (5.17) we use the formula

$$\sum_{r=1}^{\infty} \frac{(-1)^r}{r^2} = -\frac{\pi^2}{12}, \qquad (5.18)$$

so that

$$(F-N\zeta)_o = \frac{LR^2}{15\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{\infty} \frac{\partial f_o}{\partial E}\, E^{5/2}\, dE$$

$$-\frac{LR^2}{24\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2}(\beta H)^2 \int_0^\infty \frac{\partial f_0}{\partial E} E^{\frac{1}{2}} dE \tag{5.19}$$

$$-\frac{LR^2}{8\pi^3}\left(\frac{2m}{\hbar^2}\right)^{3/2}(\beta H)^2 \int_0^\infty \frac{\partial f_0}{\partial E} E^{\frac{1}{2}} dE \sum_{r=-\infty}^{\infty}{}' \frac{(-1)^r}{r^2}\, e^{\frac{\pi r E}{\beta H}}\, V_{-\frac{1}{2},0}\left(-\frac{\pi r E}{\beta H}\right),$$

where the prime on the sum indicates omission of the $r = 0$ term. So far this is exact. The conventional result[1,2] is obtained from the asymptotic formula (5.14) (for $r > 0$)

$$V_{-\frac{1}{2};0}\left(\frac{-\pi r E}{\beta H}\right) \sim \left(\frac{\beta H}{rE}\right)^{\frac{1}{2}} e^{\frac{-\pi i}{4}} . \tag{5.20}$$

Higher terms in (5.14) lead to corrections to the steady and oscillatory terms of (5.19) which contribute negligibly to the corresponding terms of the magnetic moment provided $\beta H/\zeta \ll 1$.

In evaluating $(F-N\zeta)_1$ and $(F-N\zeta)_2$ in (5.5) with the use of (5.15), we see that the $r = 0$ term in the sum can be integrated exactly, for $V_{xy}(0)$ is independent of z. This term vanishes in $(F-N\zeta)_1$, but not in $(F-N\zeta)_2$. On setting $z = \sin\theta$ for convenience and obtaining $g(z)$ and $f(z)$ from (3.13) and (3.14), we have finally

$$(F-N\zeta)_1 = \frac{LR}{\pi^2}\frac{1}{\beta H}\left(\frac{2m}{\hbar^2}\right) \int_0^\infty \frac{\partial f_0}{\partial E} E^3\, dE \;\cdot$$
$$\cdot \sum_{r=-\infty}^{\infty}{}' (-1)^r \int_{-\pi/2}^{\pi/2} \cos^2\theta \sin\theta\, d\theta\; V_{\frac{3}{2};\frac{1}{2}}\left(\frac{\pi r E}{\beta H g(\sin\theta)}\right), \tag{5.21}$$

$$(F-N\zeta)_2 = \frac{L}{105\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{1}{(\beta H)^2} \int_0^\infty \frac{\partial f_0}{\partial E} E^{7/2}\, dE$$
$$+ \frac{L}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{1}{(\beta H)^2} \int_0^\infty \frac{\partial f_0}{\partial E} E^{7/2} dE \sum_{r=-\infty}^{\infty}{}' (-1)^r \int_{-\pi/2}^{\pi/2} \sin^2\theta\cos^2\theta\, d\theta \;\cdot \tag{5.22}$$
$$\cdot\; V_{2;\frac{1}{2}}\left(\frac{\pi r E}{\beta H\, g(\sin\theta)}\right).$$

We now seek the contribution to F of states with positive values of s, whose unperturbed energies are found from (3.2) and (3.6) to be $(\hbar^2 k_z^2)/2m + (2(n+s)+1)\beta H$. If $R > 2R_c$, states perturbed appreciably by the wall have energies above the Fermi level, so that we may calculate the contribution to F with complete neglect of the wall:

$$(F-N\zeta)_+ = -kT \frac{L}{2\pi}\int_{-\infty}^{\infty} dk_z \sum_{n=0}^{\infty} \sum_{s=1}^{\infty} \ln\left(1+e^{(\zeta-(2(n+s)+1)\beta H-\frac{\hbar^2k_z^2}{2m})/kT}\right)$$

$$= \frac{2L}{3\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \int_0^{\infty} \frac{\partial f_0}{\partial E}\, dE \sum_{n=0}^{\infty} n(E-(n+\tfrac{1}{2})2\beta H)^{3/2} \qquad (5.23)$$

On setting n = n [illegible] $-\frac{1}{2}$, we can use the Poisson sum (5.7), and after some rearr[illegible]ent using (5.17) we obtain

$$(F-N\zeta)_+ = \frac{L}{\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}\int_0^{\infty} \frac{\partial f_0}{\partial E}\left\{\frac{2E^{7/2}}{105(\beta H)^2} - \frac{E^{5/2}}{15\beta H}\right\} dE$$

$$+ \frac{L}{\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}\int_0^{\infty} \frac{\partial f_0}{\partial E}\, dE \sum_{r=-\infty}^{\infty}{}' (-1)^r \left\{\frac{E^{7/2}}{6(\beta H)^2} V_{1;\frac{3}{2}}\left(\frac{\pi r E}{\beta H}\right) + \frac{iE^{3/2}}{4\pi r} V_{0;\frac{1}{2}}\left(\frac{\pi r E}{\beta H}\right)\right\}. \qquad (5.24)$$

We may now proceed most simply by using a proof given by Osborne[7] that for an electron gas in a potential field of cylindrical symmetry the volume in quantum number space bounded by a surface of constant energy and the plane $n = -\frac{1}{2}$ is independent of the field strength, at least to the accuracy of the WKB approximation,[24] and that consequently if we replace sums over quantum numbers by the appropriate integrals the resulting approximation to the free energy is independent of H. In the present discussion we have already integrated over k_z and replaced $\sum_{s=0}^{-\infty}$ in (5.1) or (5.2) by $\int_{\infty}^{0} ds$, and in the Poisson sum formula the r = 0

term arises when $\sum_{n=0}^{\infty} f(n+\frac{1}{2})$ is replaced by $\int_{-\frac{1}{2}}^{\infty} f(n+\frac{1}{2})dn$. We have moreover determined our energy eigenvalues with the WKB method. Consequently if in (5.23) we replace $\sum_{s=1}^{\infty}$ by $\int_0^{\infty} ds$ in order to make the s integration cover the range $(-\infty, \infty)$, we should expect that the sum of all the $r = 0$ terms should be independent of H. This term in $(F-N\zeta)_0$ is indeed field-independent, and this term in $(F-N\zeta)_1$ vanishes. The term arising from the mentioned modification of (5.23) is the first term in the first integral in (5.24); which combines with the $r = 0$ term in $(F-N\zeta)_2$, the first in (5.22). The sum of these two is not zero, but we recall further that we introduced an approximation in using (3.9) for the effective potential and found accordingly that ε was a function of (r_0-R) only. The exact WKB calculation yields a series of the form

$$\varepsilon = \varepsilon_0(r_0-R) + \frac{\varepsilon_1(r_0-R)}{R} + \dots \qquad (5.25)$$

Using only the first term of this series introduced no error in $(F-N\zeta)_0$, but use of the second term of (5.25) in $(F-N\zeta)_1$ yields terms of the form of $(F-N\zeta)_2$. The $r = 0$ term of this correction does in fact cancel the $r = 0$ terms of $(F-N\zeta)_2$ and $(F-N\zeta)_+$. The derivation of the second term in (5.25) is outlined in Appendix B for the purpose of obtaining important corrections to $(F-N\zeta)_2$. Osborne's theorem spares us further calculations on higher terms: we see that no $r = 0$ term will contribute to the magnetic moment.

Actually we obtained (5.24) from (5.23) by direct use of the Poisson sum without changing to an integral over s, and consequently we obtained the second term in the first integral in (5.24). This is got rid of when we note that for consistency we should have used the Poisson sum in (5.1) instead of replacing $\sum_{s=0}^{-\infty} f(s)$ by $\int_{-\infty}^{0} f(s)\,ds$. This leads to replacing the sum by $\int_{-\infty}^{\frac{1}{2}} f(s)ds$, and the extra $\int_0^{\frac{1}{2}} ds\, f(s)$ turns out to be just what is needed to cancel the second term in (5.24).

The contribution to the magnetic moment of $(F - N\zeta)_o$ and $(F - N\zeta)_+$ are immediately obtained by straightforward differentiation with respect to explicit dependence on H, with use of (5.13). From the asymptotic expansion (5.14) we find that the dominant steady and oscillatory terms are

$$M_o = \frac{LR^2}{12\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2} \beta(\beta H) \int_0^\infty \frac{\partial f_o}{\partial E} E^{\frac{1}{2}} \, dE$$

$$+ \frac{LR^2}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \beta(\beta H)^{\frac{1}{2}} \int_0^\infty \frac{\partial f_o}{\partial E} E dE \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{3/2}} \sin\left(\frac{\pi r E}{\beta H} - \frac{\pi}{4}\right), \tag{5.26}$$

$$M_+ = \frac{L}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{\beta}{(\beta H)^{3/2}} \int_0^\infty \frac{\partial f_o}{\partial E} E^2 dE \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{3/2}} \sin\left(\frac{\pi r E}{\beta H} - \frac{\pi}{4}\right)$$

$$- \frac{L}{24\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \beta \int_0^\infty \frac{\partial f_o}{\partial E} E^{\frac{1}{2}} \, dE \;. \tag{5.27}$$

To obtain the contributions of $(F - N\zeta)_1$ and $(F - N\zeta)_2$ we must use steepest descent procedures to evaluate the integrals. This is done in Appendix A; the dominant terms of the result are

$$M_1 = -\frac{LR}{2\pi^2}\left(\frac{2m}{\hbar^2}\right) \frac{\beta}{(\beta H)^{\frac{1}{2}}} \int_0^\infty \frac{\partial f_o}{\partial E} E^{3/2} \, dE \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{3/2}} \sin\left(\frac{\pi r E}{\beta H} - \frac{\pi}{4}\right)$$

$$+ \frac{LR\beta}{(\beta H)^{1/3}} \left(\frac{2m}{\hbar^2}\right)\left(\frac{3}{\pi}\right)^{\frac{1}{2}}\left(\frac{3}{2}\right)^{2/3} \frac{\Gamma(5/6)\Gamma(5/3)\zeta(5/3)\left(1 - \frac{1}{2^{2/3}}\right)}{12\pi\,\Gamma(7/3)} \cdot$$

$$\int_0^\infty \frac{\partial f_o}{\partial E} E^{4/3} \, dE, \tag{5.28}$$

$$M_2 + M_{1s} = -\frac{L}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{\beta}{(\beta H)^{3/2}} \int_0^\infty \frac{\partial f_o}{\partial E} E^2 dE \cdot \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{3/2}} \sin\left(\frac{\pi r E}{\beta H} - \frac{\pi}{4}\right)$$

$$- \frac{L\beta}{(\beta H)^{4/3}}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}\left(\frac{3}{2}\right)^{2/3} \frac{\zeta(5/3)\left(1 - \frac{1}{2^{2/3}}\right)}{81\sqrt{\pi}\,\Gamma(17/6)} \int_0^\infty \frac{\partial f_o}{\partial E} E^{11/6} \, dE, \tag{5.29}$$

where $\zeta(5/3)$ is the Riemann zeta-function. The steady term of (5.29) has been corrected to include the contribution to M_1 of the second term in (5.25), the derivation of which is sketched in Appendix B. The coefficient of the oscillatory term of (5.29) is uncorrected, for this term is too small to be of any real interest. The steady term of M_2 alone is 3/2 times the steady term of (5.29).

To contrast the magnitude of the various contributions to the moment, we have constructed Table I, in which we record the form of the dominant steady term and that of the amplitude of the dominant oscillatory term of M_0, M_1, $M_2 + M_{1s}$, and M_+, at the absolute zero of temperature, where $\partial f_0/\partial E = -\delta(E-\zeta)$. The correct numerical coefficients are given only for the steady terms in M_0, M_1, and $M_2 + M_{1s}$. We also give the condition on the radius R of the cylinder and the field strength ($R_c = \frac{c}{eH}\sqrt{2m\zeta}$) such that the steady terms in M_1, $M_2 + M_{1s}$, and M_+ are very much smaller than the steady term of M_0, the ordinary Landau diamagnetism. The condition given for the oscillatory terms is that required to make them small compared to the M_0 oscillations. Since the validity of our analysis is, as previously remarked, restricted to "strong" fields, $R >> R_c$, we see that the only significant corrections[25] to M_0 are the steady term of M_1, the so-called "surface diamagnetism" found by Osborne[7,26] and Steele,[8] and the smaller steady term of $M_2 + M_{1s}$. The numerical coefficient and temperature behavior of both are given in (5.28) and (5.29) if the integrals are evaluated. Of course, we have given only the dominant terms in the expansion of M asymptotic in $(\zeta/\beta H)$. Therefore for exceedingly high fields such that this quantity is of order unity (it can never be much less than unity except for very high temperatures), the value of M will be considerably changed. We should remark that all of our results are for a system of electrons with common spin orientation. They should be multiplied by two for a real electron gas if we continue to disregard the magnetic moment of the spin. This may be included by the method of Dingle.[19] We may thus conclude that the ordinary

Table I

	Dominant Steady Term	Dominant Oscillatory Term
M_o	$-(.02652)LR^2(\frac{2m}{\hbar^2})^{3/2}\ \beta(\beta H)\zeta^{\frac{1}{2}}$	$LR^2(\frac{2m}{\hbar^2})^{3/2}\beta(\beta H)^{\frac{1}{2}}\zeta$
M_1	$-(.02293)LR\ (\frac{2m}{\hbar^2})\ \frac{\beta}{(\beta H)^{1/3}}\zeta^{4/3}$ $R >> (\frac{\zeta}{\beta H})^{1/3}\ R_c$	$LR(\frac{2m}{\hbar^2})\ \frac{\beta}{(\beta H)^{1/2}}\ \zeta^{3/2}$ $R>>R_c$
$M_2+ M_{1s}$	$+(.004173)L(\frac{2m}{\hbar^2})^{\frac{1}{2}}\ \frac{\beta}{(\beta H)^{4/3}}\zeta^{11/6}$ $R>>(\frac{\zeta}{\beta H})^{1/6}\ R_c$	$L(\frac{2m}{\hbar^2})^{\frac{1}{2}}\ \frac{\beta}{(\beta H)^{3/2}}\zeta^2$ $R>>R_c$
M_+	$+\ L(\frac{2m}{\hbar^2})^{\frac{1}{2}}\ \beta\zeta^{\frac{1}{2}}$ $R>>(\frac{\beta H}{\zeta})^{\frac{1}{2}}R_c$	$L(\frac{2m}{\hbar^2})^{\frac{1}{2}}\ \frac{\beta}{(\beta H)^{3/2}}\ \zeta^2$ $R>>R_c$

Landau type of calculation using the free energy and neglecting the boundary states yields the correct value of the moment provided $R \gg (\zeta/\beta H)^{1/3} R_c$, and we see that the "surface diamagnetism" corrections may be obtained in a straightforward manner as well as with the elegant number theory methods of Osborne and Steele.

VI.

Corrections for Wall Thickness

We now seek the effect on the moment of the system of replacing the potential used for detailed calculations in Sections III, IV, and V, an infinite jump at radius R, by a potential that gives the wall region seen by the electrons a finite thickness. We assume the potential

$$\begin{aligned} V(r) &= \alpha(r-R)^2 \qquad &\text{for } r \geq R \\ &= 0 &\text{for } r \leq R \end{aligned} \tag{6.1}$$

and in order to simplify our work require that when $\alpha(r_1 - R)^2 = \zeta$ the "thickness" of the wall, $(r_1 - R)$, shall be very much less than the orbit radius R_c. This leads to the requirement

$$\alpha \gg \frac{e^2H^2}{2mc^2}\,. \tag{6.2}$$

In metals the wall region is probably of the order of 10^{-8} to 10^{-7} cm, and R_c is of order 10^{-3} or 10^{-4} for fields of several thousand gauss, so that the requirement (6.2) is reasonable.

We must now include the potential (6.1) in the phase integral (3.10):

$$\int_{r_1}^{R} \left[2m\left(\varepsilon - \frac{e^2H^2}{2mc^2}(r-r_o)^2\right)\right]^{\frac{1}{2}} dr + \int_{R}^{r_2} \left[2m\left(\varepsilon - \frac{e^2H^2}{2mc^2}(r-r_o)^2 - \alpha(r-R)^2\right)\right]^{\frac{1}{2}} dr$$

$$= (n + \tfrac{1}{2})\,\hbar\pi\,. \tag{6.3}$$

Changing variables with (3.13) and setting $u = (r_o - R)(\frac{eH}{\hbar c})^{\frac{1}{2}}$,

$\gamma = \frac{\alpha\hbar^2}{2m\beta^2 H^2}$, and noticing that because of (6.2) $\gamma >> 1$, we obtain on integrating and keeping only the largest of the terms involving γ

$$y = \frac{(2n+1)\pi}{\cos^{-1}z - z(1-z^2)^{\frac{1}{2}}}\left\{1 - \frac{(1-z^2)\pi}{2\,\gamma^{\frac{1}{2}}(\cos^{-1}z - z(1-z^2)^{\frac{1}{2}})}\right\}, \quad (6.4)$$

$$x = \frac{(2n+1)^{\frac{1}{2}}\sqrt{\pi}\,z}{(\cos^{-1}z - z(1-z^2)^{\frac{1}{2}})^{\frac{1}{2}}}\left\{1 - \frac{(1-z^2)\pi}{4\gamma^{\frac{1}{2}}(\cos^{-1}z - z(1-z^2)^{\frac{1}{2}})}\right\}, \quad (6.5)$$

where as usual $y = \frac{x^2}{z^2}$ to order $1/\gamma^{\frac{1}{2}}$, and $-1 \leq z \leq 1$.

We now recall that our evaluation of $(F - N\zeta)_0$ in Section V did not depend on the particular shape of the energy curve plotted against r_0, so that a potential of the present sort in no way changes the previously obtained value of $(F - N\zeta)_0$ or M_0. The only corrections come in through $(F - N\zeta)_1$ and $(F - N\zeta)_2$. We shall consider only the former, the larger one. We must then use (6.4) and (6.5) in the integral (B4) of Appendix B. We use the same device outlined there to put the integral in standard form and use the methods of Appendix A, with $\phi(\theta) = \cos^3\theta$, to evaluate it. The $r = 0$ term does not vanish but is independent of H, as we expect from Osborne's theorem. The oscillatory part of this correction to the moment is entirely negligible for the conditions we have assumed. In addition to the usual steady "surface diamagnetism" correction (5.28), however, we have the diamagnetic steady contribution

$$M_{1w} = \frac{(\frac{3}{2})^{1/3}\Gamma(\frac{4}{3})\zeta(\frac{4}{3})(1-\frac{1}{2^{1/3}})\Gamma(\frac{7}{6})}{12\sqrt{\pi}\,\Gamma(\frac{8}{3})}\,\frac{LR\beta}{\alpha^{\frac{1}{2}}}\left(\frac{2m}{\hbar^2}\right)^{3/2}(\beta H)^{1/3}\int_0^{\infty}\frac{\partial f_0}{\partial E}E^{5/3}\,dE. \quad (6.6)$$

This turns out to be small compared to the usual "surface diamagnetism" (5.28) only if

$$\alpha >> \left(\frac{\zeta}{\beta H}\right)^{2/3}\frac{e^2H^2}{2mc^2}. \quad (6.7)$$

This is a stronger condition than (6.2), but one that is satisfied in practice with a factor of 10^3 or so to spare, using the estimates for R_c and wall thickness cited above. Hence M_{1w} is negligible compared to M_1. We may infer that this conclusion is true for any other form of wall potential confined to an appropriately thin layer.

The above considerations make it appear that the susceptibility is at least for "strong" fields relatively independent of the details of the wall potential. This is true for M_o, since the calculation of this term was exact, but it is not true for M_1 for the following reason. In applying the WKB phase integral (3.5) to determine the energy eigenvalues we should, as remarked in a footnote,[17] replace $(n+\frac{1}{2})$ by $(n+3/4)$ when we assume an infinite potential wall (or equivalently the boundary condition $\psi(R) = 0$)and when the upper limit of integration in (3.5) is R. Such a replacement is dictated by WKB theory in the requirement that the phase of the approximate wave function in the classically allowed region between the turning points be such that the wave function vanishes at the turning point instead of connecting to a damped exponential in the classically forbidden region beyond the turning point, the more usual condition.[27] Similarly, if both turning points occur at infinite walls, we must use $(n+1)$ in (3.5) with $n = 0, 1, 2, \ldots$ as usual. This latter form of (3.5) in fact yields the correct eigenvalues for a one-dimensional electron in the potential $V(x) = 0$ for $|x|<a$, $V(x) = \infty$ for $|x|>a$. The $(n+3/4)$ form of (3.5) yields the exact eigenvalues for a similar problem with $V(x) = \infty$ for $x<0$, $V(x) = kx^2$ for $x>0$. Consequently if we assume an infinite potential jump at the surface of the container in the present problem, we must use $(n+3/4)$ in (3.5) when the upper turning point is at R.

At first sight one would not expect this change to make much difference, since n is quite large for most of our levels. However, it turns out that the change drastically alters the Poisson sum formula (5.7) and in this fashion alters the surface correction terms M_1 and M_2 in such a way as to produce a "surface paramagnetism"

instead of the "surface diamagnetism" found earlier. The paramagnetic result agrees with Dingle's calculations;[4] in fact our result for M_1 and M_2 using (n+3/4) agrees numerically with the terms of corresponding form and magnitude in Dingle's result (when ours are multiplied by 2 to include spin degeneracy). This is as it should be, for although Dingle begins his derivation by considering the location of the zeros of the approximate WKB wave functions, his fundamental equations are more easily derived by using (3.5) with (n+3/4) to determine the number of eigenstates of given s and k_z with energies below any given E, the turning point for such s, k_z, and E being at R.

The modified form of the Poisson sum formula is derived in Appendix C. If $0 < \alpha < 1$,

$$\sum_{n=0}^{\infty} f(n+\alpha) = \sum_{r=-\infty}^{\infty} e^{-2\pi i r\alpha} \int_{0}^{\infty} f(n)e^{2\pi i n r}dn. \qquad (6.8).$$

Using this in place of (5.7), we find we must replace the $(-1)^r$ in the sums of (5.21) and (5.22) by $e^{-2\pi i r\alpha}$. Calculation of the resulting numerical coefficients for M_1 and $M_2 + M_{1s}$ for a number of values of α between 1/2 and 3/4 yields Table II, in which the coefficients replace the bracketed numerical coefficients of Table I.

Hence the magnitude and sign of the surface corrections depend critically on the choice of α. The same is true for the value of the susceptibility at weak fields, $R \ll R_c$, calculated by Dingle.[4]

Table II

α	Coefficient M_1	Coefficient M_2+M_{1s}
.75	+ .00763	- .00139
.70	- .00047	+ .00009
.65	- .00770	+ .00140
.60	- .01378	+ .00251
.55	- .01896	+ .00345
.50	- .02293	+ .004173

As may be seen from his derivation the coefficient of this term depends on the form of the Poisson sum exactly as do the coefficients of Table II and would yield a paramagnetism roughly three times the magnitude of the reported diamagnetism if $\alpha = 1/2$ were used. All this seems contrary to what our physical intuition would lead us to expect, and we should be justified in maintaining a healthy skepticism toward the accuracy, or even the reality, of surface corrections and weak field terms calculated in this fashion from the WKB approximation. Such skepticism is especially justified if we consider the present work to be an accurate approximation to the state of affairs in an actual metal, where the surface is not sharp.

However, if we assume the reality of the surface correction and weak field susceptibility and the accuracy of the WKB method in calculating them when we assume a general wall potential more closely approximating the wall potential seen by an electron in a real metal, we must decide what value of α to choose. Certainly the wall is not infinitely sharp, so that we cannot <u>a priori</u> use $\alpha = 3/4$, but it may be sufficiently sharp so that $\alpha = 1/2$ is not sufficiently accurate for present purposes. To attempt to establish a criterion for choosing the value of α we may consider a one-dimensional electron bound by the potential

$$V(x) = \begin{cases} \infty & x < -L \\ 0 & -L < x < 0 \\ \frac{1}{2}Kx^2 & x > 0 \end{cases} \tag{6.9}$$

On one hand we shall obtain the exact solution for the energy eigenvalues, on the other the approximate WKB solution. Comparison of the two will allow us to choose the best value for α.

The exact solution for the wave function for $-L < x < 0$ and the value of the logarithmic derivative at $x = 0$ are

$$\begin{aligned} \psi(x) &= A \sin k\,(x + L) \\ \frac{\psi'(o)}{\psi(o)} &= k \cot(kL) \quad , \end{aligned} \tag{6.10}$$

where $k = \frac{1}{\hbar}(2mE)^{\frac{1}{2}}$. For $x > 0$, we must solve the equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}\chi x^2\psi = E\psi \tag{6.11}$$

subject to the boundary condition that $\psi(x)$ approaches zero as $x \to +\infty$. Making the substitutions

$$\begin{aligned} \omega &= \left(\frac{\chi}{m}\right)^{\frac{1}{2}} & E &= (n+\tfrac{1}{2})\hbar\omega \\ \alpha^4 &= \frac{m\chi}{\hbar^2} & \xi &= \alpha x \\ \psi(x) &= u(\xi) & &= \bar{H}_n(\xi)e^{-\frac{1}{2}\xi^2} \end{aligned} \tag{6.12}$$

we obtain the differential equation

$$\frac{d^2\bar{H}_n(\xi)}{d\xi^2} - 2\xi\frac{d\bar{H}_n(\xi)}{d\xi} + 2n\,\bar{H}_n(\xi) = 0 \tag{6.13}$$

This is the differential equation of the Hermite polynomials when n is integral, but we must here consider a more general n. We generalize from the well-known formula for the Hermite polynomials

$$H_n(\xi) = (-1)^n e^{\xi^2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2} = \frac{(-1)^n e^{\xi^2} n!}{2\pi i}\oint\frac{e^{-z^2}}{(z-\xi)^{n+1}}dz, \tag{6.14}$$

where the contour circles the point $z = \xi$ once counterclockwise. We find that for arbitrary n the function

$$\bar{H}_n(\xi) = \frac{e^{\xi^2}}{2\pi i}\int_C\frac{e^{-z^2}}{(z-\xi)^{n+1}}dz \tag{6.15}$$

satisfies (6.13) provided the integrand has the same value at the beginning and end of the contour. This condition and the boundary condition $u_n(\xi) = \bar{H}_n(\xi)e^{-\frac{1}{2}\xi^2} \to 0$ as $\xi \to +\infty$ are satisfied if we cut the z-plane along the real axis from $z = \xi$ to

$+\infty$, start the contour at $+\infty$ on the upper side of the cut, loop $z=\xi$ once counterclockwise, and return to $+\infty$ below the cut. It is now easy to evaluate $\bar{H}_n(0)$ and $\left.\frac{d\bar{H}_n(\xi)}{d\xi}\right|_{\xi=0}$ by substituting $t=z^2$. The contour D in the t-plane corresponding to C makes use of two Riemann surfaces in looping the origin twice but it may be deformed into two loops around the origin, each stretching out to $+\infty$ on the real axis. We may now replace this contour by C', which has the form C had in the z-plane, and we now use a single Riemann surface cut from the origin to $+\infty$ along the real axis but traverse C' twice, the phase of the integrand on the second circuit being advanced over that of the first circuit by the difference in phase of the integrand on the two sides of the cut. The value of the resulting contour integral is now obtained immediately from Hankel's integral for the gamma-function.[28]

$$\bar{H}_n(o) = \frac{e^{-\pi i n}\cos\frac{\pi n}{2}}{\Gamma(1+n/2)}$$
$$\bar{H}_n'(o) = \frac{2e^{-\pi i n}\sin\frac{\pi n}{2}}{\Gamma(\frac{1}{2}+n/2)} \tag{6.16}$$

We may therefore obtain the logarithmic derivative of the wave function at the origin

$$\frac{\psi'(o)}{\psi(o)} = \frac{\bar{H}_n'(o)}{\bar{H}_n(o)}\frac{d\xi}{dx} = 2\left(\frac{m\chi}{\hbar^2}\right)^{1/4}\tan\frac{\pi n}{2}\,\frac{\Gamma(\frac{n}{2}+1)}{\Gamma(\frac{n}{2}+\frac{1}{2})} \tag{6.17}$$

Equating this to (6.10), we obtain the equation for E whose roots yield the eigenvalues:

$$k\cot kL = 2\left(\frac{m\chi}{\hbar^2}\right)^{1/4}\tan\frac{\pi n}{2}\,\frac{\Gamma(\frac{n}{2}+1)}{\Gamma(\frac{n}{2}+\frac{1}{2})} \tag{6.18}$$

For the WKB solution we use the phase integral condition

$$(s+a)\pi\hbar = L(2mE)^{\frac{1}{2}} + \int_0^{x_1}[2m(E-\tfrac{1}{2}\chi x^2)]^{\frac{1}{2}}\,dx \tag{6.19}$$

where s is a positive integer and we consider E to be some root of (6.18) and α to be some number between zero and one which makes (6.19) exact. Integrating (6.19) and using (6.12), we find

$$(s+\alpha)\,\pi = kL + (2n+1)\,\frac{\pi}{4}\ . \tag{6.20}$$

We now use (6.20) and (6.12) to find that

$$\cot kL = \cot\left\{(s+\alpha)\,\pi - \frac{\pi E}{2\hbar\omega}\right\} = \cot\left\{\pi\alpha - \frac{\pi E}{2\hbar\omega}\right\}. \tag{6.21}$$

Substituting this in (6.18), we obtain

$$\cot\left\{\pi\alpha - \frac{E\pi}{2\hbar\omega}\right\} = \left(\frac{2\hbar\omega}{E}\right)^{\frac{1}{2}} \frac{\Gamma\left(\frac{E}{2\hbar\omega} + \frac{3}{4}\right)}{\Gamma\left(\frac{E}{2\hbar\omega} + \frac{1}{4}\right)} \cot\left\{\frac{3\pi}{4} - \frac{E\pi}{2\hbar\omega}\right\}. \tag{6.22}$$

We now assume that L is large enough so that the spacing of the eigenvalues of the system is small compared to $\hbar\omega$, so that we may regard E in (6.20), which really denotes an eigenvalue, as a variable with a continuous range. We then solve (6.21) for α as a function of $E/\hbar\omega$. Values at representative points are given in Table III.

<u>Table III</u>

$E/\hbar\omega$	α
$\to \infty$	$\to 3/4$
6	.750
2	.753
1	.743
1/2	.750
1/10	.838
1/100	.938
$\to 0$	$\to 1$

We see that provided $E/\hbar\omega > 1/2$, α is remarkably close to 3/4. We may therefore expect for the WKB solution to the problem of the electron in a box in a magnetic field that α will be close to 1/2 provided $E/\hbar\omega > 1/2$, since in this instance the potential is slowly

varying at the other turning point in contrast to the above model. Approximating the wall potential in an actual metal as in (6.1) by $\frac{1}{2}\varkappa(r - R)^2$, and defining $\varkappa$ in terms of the wall thickness $(r_1 - R)$ and the Fermi energy ξ by $\frac{1}{2}\varkappa(r_1 - R)^2 = \xi$, we find

$$\frac{\xi}{\hbar\omega} = \frac{(r_1-R)}{\hbar}\left(\frac{\xi m}{2}\right)^{\frac{1}{2}}. \qquad (6.23)$$

Using $\xi \sim 10^{-12}$ erg. $(r_1 - R) \sim 10^{-8}$cm, and the free electron mass, we find $\frac{\xi}{\hbar\omega} \sim 1/10$. Comparing this with Table III we see that this puts us in the critical region with an intermediate value of α, especially since most occupied states have energies below ξ. However, we see from this that ξm has to be quite small before we get into the "sharp wall region" where $\alpha = 3/4$ in the magnetic problem, and we see from Table II that in the intermediate region the dominant surface correction M_1 is diamagnetic (and Dingle's weak field susceptibility is paramagnetic), although not so large as we found previously using $\alpha = 1/2$. This suggests that provided the periodic potential doesn't alter the situation too drastically in a real metal, the surface correction M_1 is diamagnetic. However, skepticism of the accuracy of all these susceptibility calculations seems justified.

Finally, we may remark that the theorem proved by Osborne (Section V) requires slight modification when $(n+\frac{1}{2})$ is replaced by $(n+\alpha)$ in the calculation of the energy eigenvalues by the WKB method. As may be seen from Osborne's proof, the volume in quantum-number space that is invariant is now bounded by the plane $n = -\alpha$ instead of $n = -\frac{1}{2}$. Fortunately, this is the natural generalization, since the modified Poisson sum (6.8) leads us to replace $\sum_{n=0}^{\infty} f(n+\alpha)$ by $\int_{-\alpha}^{\infty} f(n+\alpha)dn$ in the $r = 0$ term.

VII.

The Harmonic Oscillator Model of Darwin

We have heretofore required that $V(r)$ be constant except for a

3

rapid rise at the wall. That the results can be quite different when the boundary is extended is shown by the following results on Darwin's model. These are of no importance in the interpretation of experimental results, as the model is rather unrealistic, but they are given for curiosity's sake, since the problem seems to be the only one that can be solved more or less exactly for all ranges of field strength, as well as to show that contrary to intimations in the literature Darwin's model does not give the same results as the electron-in-a-box model when Fermi statistics are used. Hence it should be used with care if used at all as a guide to thought.

Following Darwin,[10] we consider a system of electrons bound by the potential of the two-dimensional harmonic oscillator: $V = \frac{1}{2} m\omega^2(x^2+y^2)$. We first use an approximate procedure for strong fields to show some interesting features. We choose ω such that $\hbar\omega \ll \beta H$ for $H \geq H_0$. Then we may show that with neglect of the spin the energies of individual states are to a sufficiently accurate approximation for $H \geq H_0$

$$\varepsilon_{n,m',k_z} = (2n+1)\beta H + m'\frac{\hbar^2\omega^2}{2\beta H} + \frac{\hbar^2 k_z^2}{2m}, \qquad \begin{array}{l} 0 \leq n < \infty, \\ -n \leq m' < \infty, \end{array} \tag{7.1}$$

where n, m', k_z and spin orientation form a complete set of quantum numbers.

If now we consider a "two-dimensional" system of electrons with a common value of k_z, it proves quite easy to sum the moments of the lowest N states to get the total moment of the system at absolute zero. This is sketched in Fig. III as a function of the parameter γ^2 related to H by

$$H^2 = \frac{N\hbar^2\omega^2}{2\beta^2}\gamma^2 . \tag{7.2}$$

This is qualitatively different from the results for the electrons in a box in that the system never becomes paramagnetic and the amplitude of oscillation decreases as H decreases. Moreover, for $\gamma^2 \ll 1$, the local average of the moment is

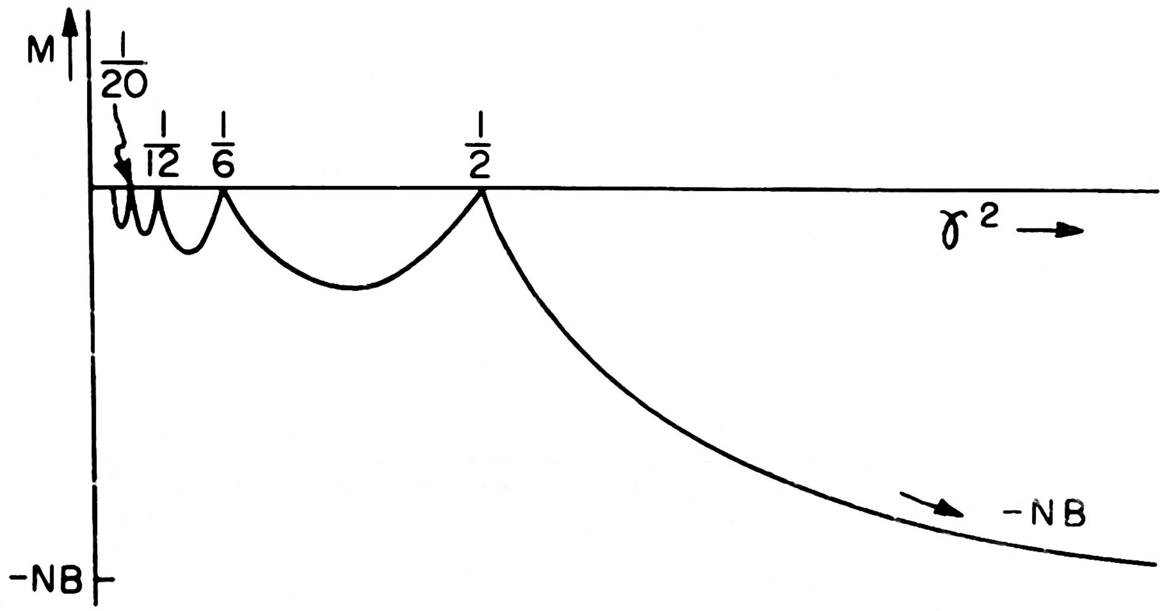

FIG. III MAGNETIC MOMENT OF A TWO-DIMENSIONAL SYSTEM OF ELECTRONS IN OSCILLATOR POTENTIAL AT $T = 0°$ K. SPIN IS NOT INCLUDED. (SEE EQUATION (7.2) OF TEXT FOR DEFINITION OF γ^2

$$\overline{M} = \frac{-n(\zeta)\, \beta^2 H}{3} , \qquad (7.3)$$

where $n(\zeta)$ represents the density of states at the Fermi level. In the box problem the average moment is zero for the two-dimensional model. We can add the average moments (7.3) for systems of electrons with different values of k_z and get the result in the same form, with $n(\zeta)$ the total density of states at the Fermi level of a three-dimensional system. This is now formally exactly the same as one of the forms of Landau's result for free electrons in three dimensions given in (2.6). Of course, $n(\zeta)$ is different in the two problems and in particular depends on ω here. The harmonic oscillator model also leads to low temperature oscillations in the susceptibility per electron of the complete system, as plotted for absolute zero in Fig. IV. Again the curve differs from that for the system of electrons in a box,[11,12] in having the oscillations smooth and much smaller in magnitude than the Landau average value. In Fig. V the susceptibility is plotted when the contribution of the spin to the moment is included.

The curves of Figs. IV and V were plotted from numerical calculations at absolute zero. We now turn to a new derivation for finite temperatures and arbitrary field strengths, which will be a slight modification of the method recently introduced by Sondheimer and Wilson (S-W).[2]

Following S-W, we seek first to evaluate the classical partition function $Z(\gamma)$, where $\gamma = 1/kT$:

$$Z(\gamma) = \sum_{l} e^{-\gamma E_l} . \qquad (7.4)$$

The Schrödinger equation for the Darwin model is (3.1) with E replaced by $(E - \frac{1}{2}m\,\omega^2(x^2+y^2))$. We let our system have length L in the direction parallel to the field. The energy eigenvalues are

$$E_{n,s,k_z} = (2n + |s| + 1)(\beta^2 H^2 + \hbar^2\omega^2)^{\frac{1}{2}} + s\,\beta H + \frac{\hbar^2 k_z^2}{2m} , \qquad (7.5)$$

$$n = 0,1,2,\ldots\ , \quad s = 0, \pm 1, \pm 2, \ldots\ .$$

The approximate values (7.1) may be obtained from (7.5) when $\hbar\omega \ll \beta H$.

We assume L large enough so that we may replace the sum over k_z by an integral. Then

$$Z(\gamma) = \sum_{n,s} e^{-\gamma[2n+|s|+1)\tau + s\beta H]}\ \frac{L}{2\pi}\int_{-\infty}^{\infty} e^{-\gamma\frac{\hbar^2 k_z^2}{2m}}\, dk_z$$

$$= L\left(\frac{2\pi m}{\gamma h^2}\right)^{\frac{1}{2}} \sum_{n=0}^{\infty}\sum_{s=-\infty}^{\infty} e^{-\gamma[2n+|s|+1)\tau + s\beta H]}\ , \tag{7.6}$$

where $\tau = (\beta^2 H^2 + \hbar^2\omega^2)^{\frac{1}{2}}$.

The sums over n and s are easily done, and the result is

$$Z(\gamma) = \frac{L}{4}\left(\frac{2\pi m}{\gamma h^2}\right)^{\frac{1}{2}} \frac{1}{\sinh[\frac{\gamma}{2}(\tau-\beta H)]\sinh[\frac{\gamma}{2}(\tau+\beta H)]}\ . \tag{7.7}$$

It is an interesting verification of Dingle and Osborne's theorem (Section V and Reference 24) that if in (7.6) we replace sums over n and s by integrals, the integration limits for s being $(-\infty, \infty)$, and those for n $(-\frac{1}{2}, \infty)$, then $Z(\gamma)$ turns out to be independent of H. If the n lower limit n_o is anything other than $-\frac{1}{2}$, however, $Z(\gamma)$ depends on H through the factor $e^{-\gamma\tau(2n_o+1)}$. The value $n_o = -\frac{1}{2}$ occurs automatically in the Poisson sum formula and is required in Osborne's proof.

We now use directly S-W's conclusion that the free energy for Fermi statistics is given by

$$F - N\zeta = \int_0^{\infty} \frac{\partial f_o}{\partial E}\, z(E)\,dE, \tag{7.8}$$

where f_o is the usual Fermi function and

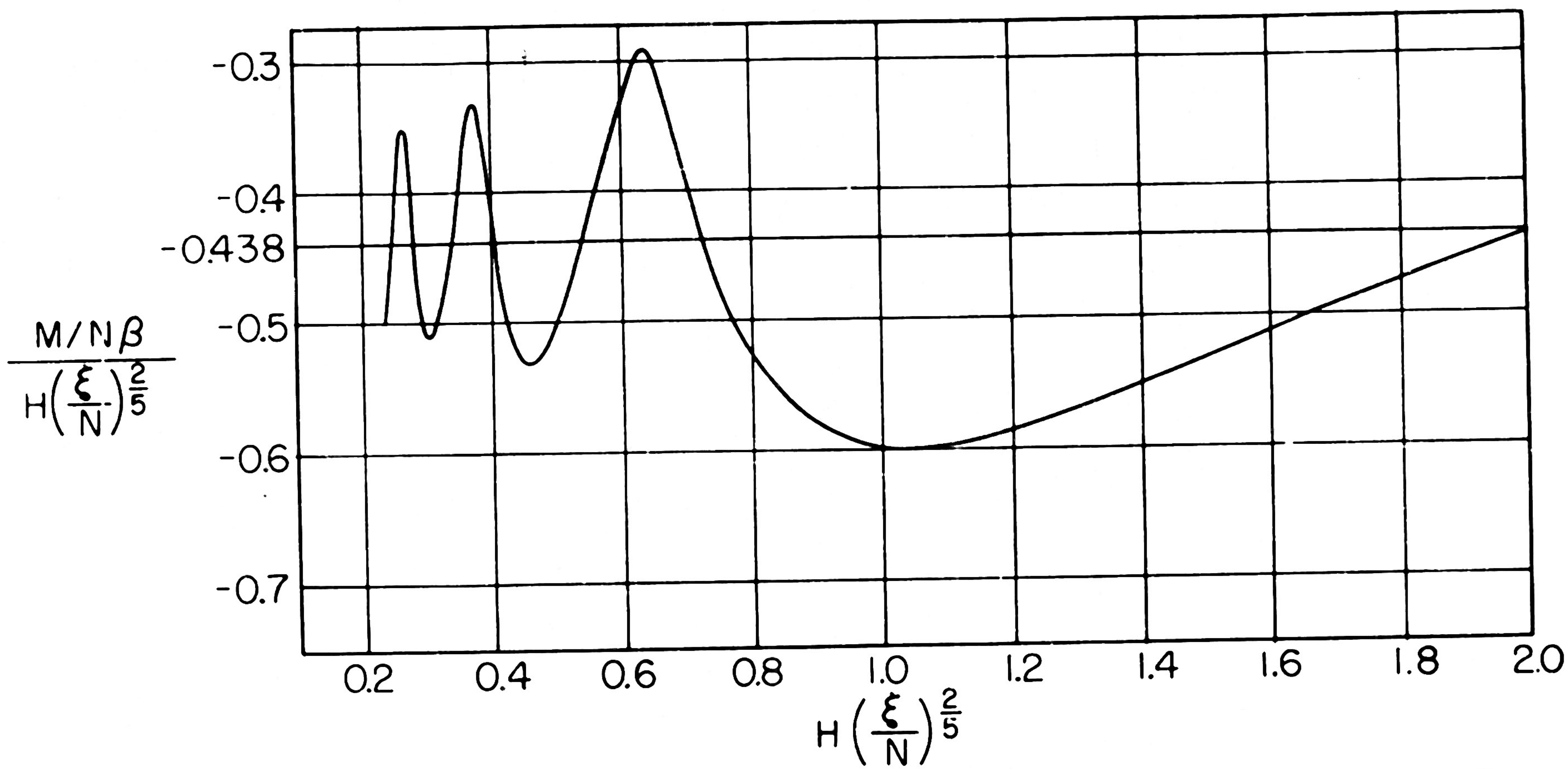

FIG. IV SUSCEPTIBILITY OF A THREE-DIMENSIONAL SYSTEM OF ELECTRONS IN OSCILLATOR POTENTIAL AT $T=0°K.$, FOR FIELD STRENGTHS SUCH THAT $\zeta/2\beta H$ IS OF ORDER UNITY. SPIN IS NOT INCLUDED. THE HORIZONTAL LINE INDICATES THE VALUE OF THE LANDAU STEADY DIAMAGNETISM FOR LOW FIELD STRENGTHS. THE QUANTITY ξ IS DEFINED TO BE

$$\frac{4\beta^{\frac{5}{2}} L \sqrt{2M}}{3\pi \hbar^3 \omega^2}$$

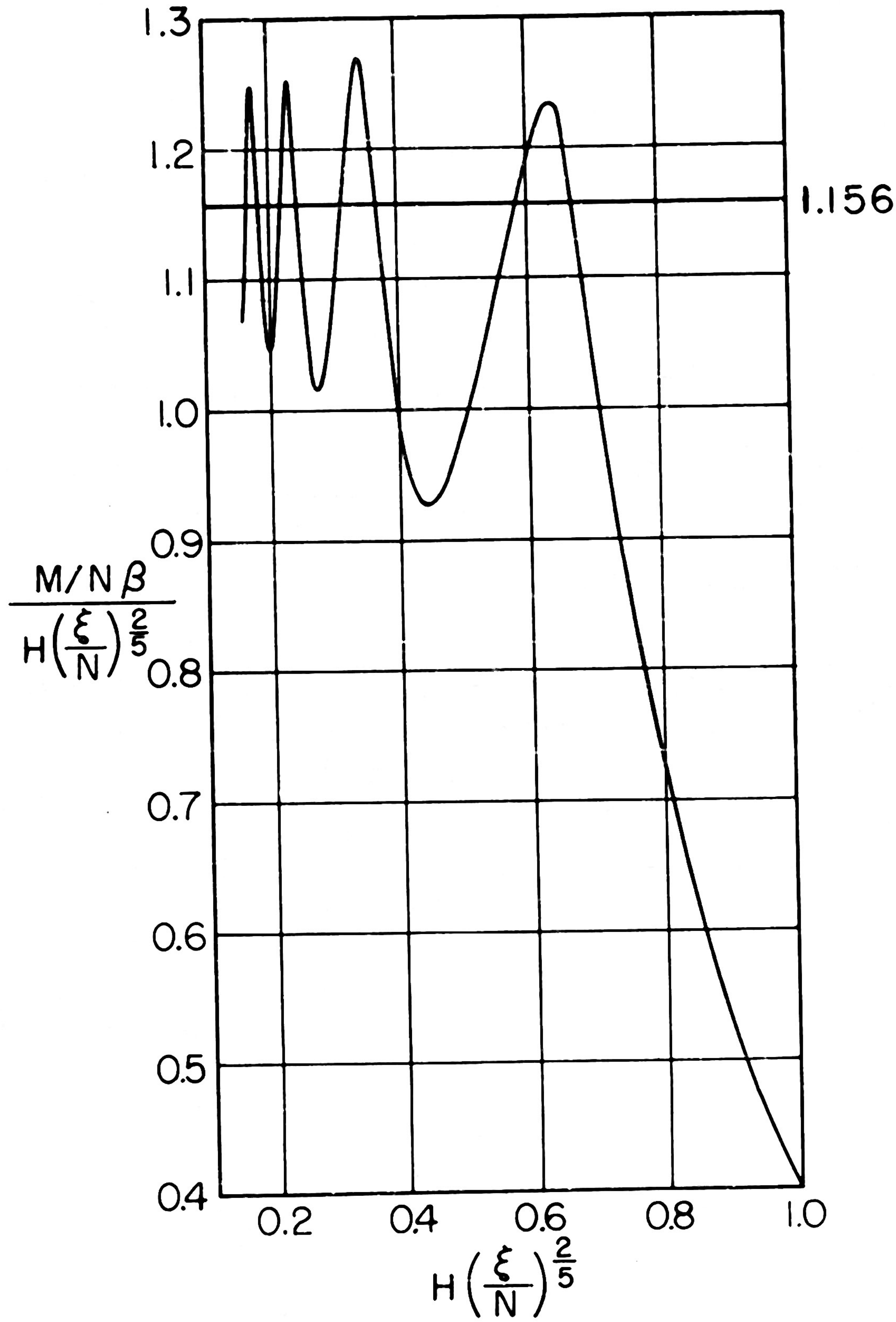

FIG. V SAME AS FIG. IV, BUT WITH MOMENT OF SPIN INCLUDED

$$z(E) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{E\lambda}\,\frac{Z(\lambda)}{\lambda^2}\,d\lambda\ , \qquad (7.9)$$

the path of integration being to the right of all singularities of the integrand. As before, our results are for electrons with a common spin orientation.

The integral (7.9) is evaluated in a straightforward manner by the method of S-W. As in S-W, the poles of the integrand contribute the oscillatory part of $z(E)$, the integral around the branch point at the origin the steady part. The general result is

$$z(E) = L\left(\frac{2\pi m}{h^2}\right)^{\frac{1}{2}}\left\{\frac{1}{4}\sum_{\alpha=1,2}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2\pi n)^{5/2}}\,\frac{(\tau+(-1)^{\alpha}\beta H)^{3/2}}{\sin\left[\frac{\pi m}{\hbar^2\omega^2}(\tau-(-1)^{\alpha}\beta H)^2\right]}\right.$$

$$\cdot\ \sin\left(\frac{2\pi m E}{\tau+(-1)^{\alpha}\beta H}-\frac{\pi}{4}\right) \qquad (7.10)$$

$$\left.+\ \frac{E^{7/2}}{\hbar^2\omega^2\,\Gamma(9/2)}-\frac{1}{12}\left(1+2\,\frac{\beta^2H^2}{\hbar^2\omega^2}\right)\frac{E^{3/2}}{\Gamma(5/2)}+\cdots\right\},$$

where higher terms in the asymptotic expansion of the steady part are small provided $E/\beta H \gg 1$, $E/\hbar\omega \gg 1$.

For high fields, $\beta H \gg \hbar\omega$, we can most simply obtain the dominant terms of (7.10) by replacing $\sinh \frac{\lambda}{2}(\tau-\beta H)$ in (7.7) by $\frac{\lambda}{2}(\tau-\beta H)$ and integrating (7.9) anew. Using this result to calculate the moment, as in S-W, we find with neglect of small temperature-dependent corrections that the dominant terms are, in terms of $n(\zeta)$, the density of states at the Fermi level,

$$\frac{M}{H} = \frac{-n(\zeta)\beta^2}{3}+\frac{3}{2}n(\zeta)\beta^2\left(\frac{kT}{\beta H}\right)\left(\frac{\beta H}{\zeta}\right)^{\frac{1}{2}}\sum_{r=1}^{\infty}\frac{(-1)^r}{r^{3/2}}\,\frac{\cos\left(\frac{\pi r\zeta}{\beta H}-\frac{\pi}{4}\right)}{\sinh\left(\frac{\pi^2 kTr}{\beta H}\right)}\ , \qquad (7.11)$$

which may be contrasted with the usual result[1] for electrons in a box, with the appropriate $n(\zeta)$

$$\frac{M}{H} = -\frac{n(\zeta)\beta^2}{3} + n(\zeta)\beta^2\pi\left(\frac{kT}{\beta H}\right)\left(\frac{\zeta}{\beta H}\right)^{\frac{1}{2}}\sum_{r=1}^{\infty}\frac{(-1)^r}{r^{\frac{1}{2}}}\frac{\sin\left(\frac{\pi r\zeta}{\beta H}-\frac{\pi}{4}\right)}{\sinh\left(\frac{\pi^2 kTr}{\beta H}\right)} . \qquad (7.12)$$

The principal differences are in the phase and amplitude of the oscillations. Thus the amplitude in (7.11) varies as $\left(\frac{\beta H}{\zeta}\right)^{\frac{1}{2}}$, whereas that of (7.12) varies as the reciprocal of this and is therefore much larger than the Landau steady term for sufficiently low temperature.

For fields low enough so that $\frac{\beta H}{\hbar\omega} \ll 1$, but large enough so that $\frac{\zeta\beta H}{\hbar^2\omega^2} \gg 1$, we obtain from (7.10) the dominant terms

$$\frac{M}{H} = -\frac{n(\zeta)\beta^2}{3} - \frac{3}{16\sqrt{2}}\, n(\zeta)\,\beta^2\left(\frac{\hbar\omega}{\zeta}\right)^{\frac{1}{2}}\left(\frac{\hbar\omega}{\beta H}\right)\left(\frac{kT}{\beta H}\right) \cdot$$

$$\cdot \sum_{n=1}^{\infty}\frac{\cos\left(\frac{2\pi n\zeta}{\hbar\omega}-\frac{\pi}{4}\right)\cos\left(\frac{2\pi n\beta H\zeta}{\hbar^2\omega^2}\right)}{n^{3/2}\sinh\left(\frac{2\pi^2 kTn}{\hbar\omega}\right)} \qquad (7.13)$$

For very weak fields such that $\frac{\zeta\beta H}{\hbar^2\omega^2} \ll 1$, we have finally

$$\frac{M}{H} = \frac{-n(\zeta)\beta^2}{3} - \frac{15\pi}{32\sqrt{2}}\, n(\zeta)\,\beta^2\left(\frac{kT}{\hbar\omega}\right)\left(\frac{\zeta}{\hbar\omega}\right)^{\frac{1}{2}} \cdot$$

$$\cdot \sum_{n=1}^{\infty}\frac{\sin\left(\frac{2\pi n\zeta}{\hbar\omega}-\frac{\pi}{4}\right)}{n^{\frac{1}{2}}\sinh\left(\frac{2\pi^2 kTn}{\hbar\omega}\right)} . \qquad (7.14)$$

The last term in (7.14) arises from the oscillatory terms of (7.10) in the limit as $\beta H \to 0$. We see that it is much larger than the true steady susceptibility $\frac{-n(\zeta)\beta^2}{3}$ for such weak fields and sufficiently low temperature but that its sign and magnitude

depend critically on the ratio $\xi/\hbar\omega$.

We note from (7.10) that the ordinary Landau susceptibility is the dominant steady term for all but exceedingly weak fields. This contrasts with Dingle's finding that electrons in a box show a steady susceptibility considerably larger than the Landau value, for weak fields comparable to those required for the validity of (7.13). This contrasts also with the importance of the "surface diamagnetism" for the box model at intermediate fields. However, the oscillatory terms in (7.13) are quite similar to the oscillatory terms in Dingle's weak field calculations[4] if we identify the "radius" R of our system by setting $\xi = \frac{1}{2}m\omega^2R^2$.

Appendix A.

From (5.21) and (5.22) we see that we must evaluate integrals of the form

$$\int_{-\pi/2}^{\pi/2} \phi(\theta) V_{xy}\left(\frac{\omega}{g(\sin\theta)}\right) d\theta = \int_0^1 u^x(1-u)^y du \int_{-\pi/2}^{\pi/2} \phi(\theta) e^{\frac{i\omega u}{\pi} h(\theta)} d\theta, \tag{A1}$$

in which we have used (5.9), have written $\omega = \frac{\pi r E}{\beta H}$, and have from (3.14) $h(\theta) = \frac{\pi}{2} - \theta - \sin\theta\cos\theta$. Here $\phi(\theta)$ is $\cos^2\theta\sin\theta$ or $\cos^2\theta \sin^2\theta$. If $\phi(\theta) = \cos^2\theta$, as in the R^2 term of (5.4) in (5.3), then since $\frac{dh}{d\theta} = -2\cos^2\theta$, we see from (5.13) that the integral is exactly integrable. In general we must resort to an approximate evaluation asymptotic in ω. The following procedure does not yield the complete asymptotic expansion of (A1) but gives enough of it for our present purposes.

The integral in (A1) is of the form approximated by Steele[29] with van der Corput's method of critical points.[30] However, the ultimate justification of this procedure in this problem seems to be the method of steepest descent, since for $n \geq m-1$, an integral of the form $\int_0^\infty x^n e^{i|y|x^m} dx$ does not converge if the path of integration is the real axis. Since we shall have to avoid divergences resulting from terms in $(\omega u)^{-k}$, with $k \geq x+1$, in the asymptotic expansion of the inner integral in (A1) when the u integration is carried out, we should justify our procedure carefully and to this end can most conveniently use the method of steepest descent directly. The following discussion is tailored to the particular $\phi(\theta)$, $h(\theta)$ in our problem.

We now regard $\phi(\theta)$ and $h(\theta)$ as analytic functions of the complex variable θ. From the imaginary part of $h(\theta)$ we find that for $\omega u > 0$ the path of integration of the inner integral in (A1) should be deformed into the "steepest" path $\gamma_1 + \gamma_2$ sketched

in Fig. VI. The complete asymptotic development of the inner integral is then obtained by expanding $\phi(\theta)$ and $h(\theta)$ about the critical points $\theta_1 = -\frac{\pi}{2}$, $\theta_2 = \frac{\pi}{2}$, where $\left| e^{\frac{i\omega u}{\pi} h(\theta)} \right|$ assumes its greatest value (unity) on the path $\gamma_1 + \gamma_2$:

$$\sum_{i=1,2} e^{\frac{i\omega u}{\pi} h(\theta_i)} \int_{\gamma_i} \left(\sum_{k=0}^{\infty} \frac{\phi^{(k)}(\theta_i)(\theta-\theta_i)^k}{k!} \right) e^{\frac{i\omega u}{\pi} \frac{h^{(m)}(\theta_i)(\theta-\theta_i)^m}{m!}} \tag{A2}$$

$$\cdot \sum_{P=0}^{\infty} \left(\frac{i\omega u}{\pi} \sum_{s=1}^{\infty} \frac{h^{(m+s)}(\theta_i)(\theta-\theta_i)^{m+s}}{(m+s)!} \right)^P \frac{1}{P!} \, d\theta,$$

where $h^{(m)}(\theta_i)$ is the first non-zero derivative of $h(\theta_i)$ (for our problem the third). Each term in the expansion is evaluated asymptotically (such that $(\omega u)^n$ times the error in each term approaches zero as $(\omega u) \to \infty$ for all n) by replacing γ_i by the rectilinear path μ_i tangent to γ_i at θ_i and taken in the same sense. The general result from terms with p = 0,1 is that given by Steele in his equations (A9) and (A10).[8]

Using the special form of $h(\theta)$, $\phi(\theta)$ in our problem (Table IV), the interesting terms of (A2) are those involving $\phi^{(2)}(\theta_i)$, $\phi^{(4)}(\theta_i)$ and $\phi^{(2)}(\theta_i)h^{(5)}(\theta_i)$, at both $\pm\frac{\pi}{2}$.

Since $h^{(3)}(\pm\frac{\pi}{2}) = -4$ and

$$\int_{\infty\,(\mu_2)}^{\pi/2} (\theta - \tfrac{\pi}{2})^n e^{\frac{-2i\omega u}{3\pi}(\theta - \frac{\pi}{2})^3} d\theta \sim \left(\frac{3\pi}{2\omega u}\right)^{\frac{n+1}{3}} \frac{(-1)^n e^{\frac{(n+1)\pi i}{6}}}{3} \Gamma\left(\frac{n+1}{3}\right) \tag{A3}$$

for $\omega u > 0$, (with the corresponding equation at $-\frac{\pi}{2}$), we have for the first two terms at $\pm\frac{\pi}{2}$ for the inner integral in (A1) with $\phi(\theta) = \cos^2\theta \sin\theta$ and $\omega u > 0$

$$\sim \left\{ \frac{\pi i}{2\omega u} - \frac{1}{6}\left(\frac{3\pi}{2\omega u}\right)^{5/3} e^{\frac{5\pi i}{6}} \Gamma(5/3) \right\} \tag{A4}$$

$$+ e^{i\omega u} \left\{ \frac{\pi i}{2\omega u} + \frac{1}{6}\left(\frac{3\pi}{2\omega u}\right)^{5/3} e^{\frac{-5\pi i}{6}} \Gamma(5/3) \right\}.$$

For $\omega u < 0$ we obtain the development by conjugation, as with the asymptotic formula (5.14). A similar expansion holds for $\phi(\theta) = \cos^2\theta\sin^2\theta$.

This expansion of the inner integral, which we shall call $\psi(\omega u)$, in (A1) is asymptotic in ωu, but since the integral over u extends down to $u = 0$ we must make certain that the result after the u integration is asymptotic in ω. Since a term in $(1/u)^k$ in (A4), with $k \geq x + 1$, leads to a divergent u integral, we see, as remarked above, that we can at best obtain by this method no more than the first few terms of the complete asymptotic development of the double integral (A1).

We accordingly assume an asymptotic approximation to $\psi(\omega u)$ of the form

$$\xi(\omega u) = \frac{\alpha(\omega u)}{(\omega u)^k} , \tag{A5}$$

where $k < x + 1$ and $|\alpha(\omega u)| < c$, a constant, for all ωu, such that for an arbitrary $\delta > 0$, there exists an A such that whenever $\omega u \geq A$

$$|\psi(\omega u) - \xi(\omega u)| \ (\omega u)^k < \delta . \tag{A6}$$

(The proof is readily extended to a more general expansion of $\xi(\omega u) = \sum_{i=1}^{n} \frac{\alpha_i(\omega u)}{(\omega u)^{k_i}}$, provided that all the $k_i < x + 1$.) Then if $u \geq \varepsilon$ and $\omega \geq A/\varepsilon$, (A6) will be satisfied. Moreover for either of the $\phi(\theta)$ of interest to us, $|\psi(\omega u)| < \pi$. Accordingly,

$$\left|\int_0^1 (\psi(\omega u) - \xi(\omega u))u^x(1-u)^y du\right| \omega^k \leq \omega^k \left|\int_0^{\varepsilon} \psi(\omega u)u^x(1-u)^y \, du\right|$$

$$+ \omega^k \left|\int_0^{\varepsilon} \xi(\omega u)u^x(1-u)^y du\right| + \omega^k \left|\int_{\varepsilon}^1 \left|\psi(\omega u) - \xi(\omega u)\right| u^x(1-u)^y du\right|$$

$$\leq \omega^k \pi \int_0^{\varepsilon} u^x du + c \int_0^{\varepsilon} u^{x-k} du + \delta \int_{\varepsilon}^1 u^{x-k} \, du$$

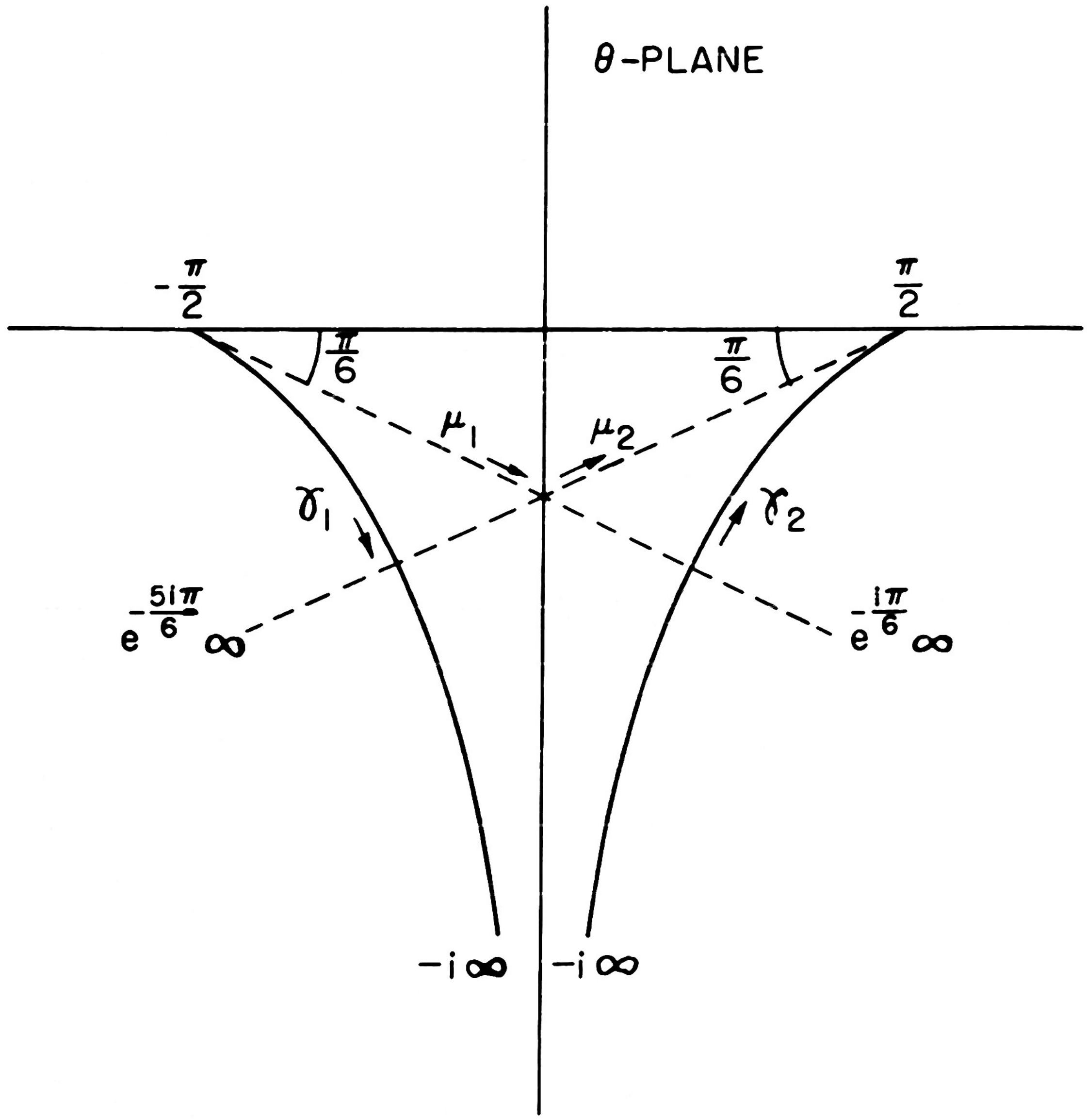

FIG. VI CONTOUR OF INTEGRATION FOR (A2)

$$= \frac{\pi \omega^k \varepsilon^{x+1}}{x+1} + \frac{(c-\delta)\varepsilon^{x-k+1}}{(x-k+1)} + \frac{\delta}{(x-k+1)} . \qquad (A7)$$

By choosing

$$\varepsilon = \left(\frac{1}{\omega}\right)^{\frac{k}{x+1-\lambda}} , \qquad \text{where} \quad \lambda = \tfrac{1}{2}(x+1-k) > 0, \qquad (A8)$$

we may determine A such that $\frac{\delta}{x-k+1} < \eta/3$, where $\eta > 0$ is arbitrarily small. We may then choose ω such that the first two terms in (A7), which according to (A8) each vary as a negative power of ω, are each less than $\eta/3$, and simultaneously

$$(\omega)^{\frac{x+1-k-\lambda}{x+1-\lambda}} \geq A, \qquad (A9)$$

which suffices to make $\omega \geq A/\varepsilon$. Hence for sufficiently large ω

$$\omega^k \left| \int_0^1 (\psi(\omega u) - \xi(\omega u))\, u^x (1-u)^y du \right| < \eta ,$$

so that substitution of (A4) yields the asymptotic expansion of (A1) through terms with $k < x + 1$, but we have no assurance that higher terms are given accurately, even if they do not diverge. Substitution of (A4) yields then for (A1)

$$\sim \frac{\pi i}{2\omega} V_{x-1;y}(\omega) + \frac{1}{6}\left(\frac{3\pi}{2\omega}\right)^{5/3} e^{\frac{-5\pi i}{6}} \Gamma(5/3)\, V_{x-\frac{5}{3};y}(\omega)$$

$$+ \frac{\pi i}{2\omega} V_{x-1;y}(0) - \frac{1}{6}\left(\frac{3\pi}{2\omega}\right)^{5/3} e^{\frac{5\pi i}{6}} \Gamma(5/3)\, V_{x-\frac{5}{3};y}(0) , \qquad (A10)$$

and we must use (5.14) to eliminate terms varying as $(1/\omega)^k$ with $k \geq x + 1$. For (5.21) we see that this condition actually eliminates all the oscillatory terms, so that the oscillatory term in (5.28) may be inaccurate. We know at least that it is no larger than the order of magnitude there given, so that Table I assures us that it is certainly negligible.

The dominant term in(A10) is the third one, but this vanishes

Appendix B.

In order to calculate the second term of (5.25) and the correction to $(F-N\zeta)_1$, we must include the next term, $-\frac{e^2H^2}{2mc^2r_o}(r-r_o)^3$ of the expansion (3.9) in the phase integral (3.10). We then change variables to x and y of (3.13) and set $u = (r_o-r)(\frac{eH}{\hbar c})^{\frac{1}{2}}$. Making the further substitutions

$$v = u\left(1 + \frac{u}{2(\frac{eH}{\hbar c})^{\frac{1}{2}}r_o}\right) \quad \text{and} \quad v_x = x\left(1 + \frac{x}{2(\frac{eH}{\hbar c})^{\frac{1}{2}}R}\right),$$

we obtain for the phase integral

$$\int_{v_x}^{v_1}(y-v^2)^{\frac{1}{2}}\left(1 - \frac{v}{(\frac{eH}{\hbar c})^{\frac{1}{2}}R}\right)dv = (n+\tfrac{1}{2})\pi, \tag{B1}$$

where $y = v_1^2$, and (B1) is accurate through terms in $1/R$. Introducing the parameter $z = v_x/y^{\frac{1}{2}}$, which has the range $-1\leq z\leq 1$, we obtain the equations replacing (3.14) by integrating:

$$y = \frac{(2n+1)\pi}{\cos^{-1}z-z(1-z^2)^{\frac{1}{2}}}\left\{1 + \frac{\frac{2}{3}(2n+1)^{\frac{1}{2}}\sqrt{\pi}\,(1-z^2)^{3/2}}{(\frac{eH}{\hbar c})^{\frac{1}{2}}R\,(\cos^{-1}z-z(1-z^2)^{\frac{1}{2}})^{3/2}},\right\} \tag{B2}$$

$$x = \frac{(2n+1)^{\frac{1}{2}}\pi z}{(\cos^{-1}z-z(1-z^2)^{\frac{1}{2}})^{\frac{1}{2}}}\left\{1 - \frac{(2n+1)^{\frac{1}{2}}\sqrt{\pi}}{(\frac{eH}{\hbar c})^{\frac{1}{2}}R}\,\frac{\left\{\frac{1}{2}z(\cos^{-1}z-z(1-z^2)^{\frac{1}{2}})-\frac{1}{3}(1-z^2)^{\frac{3}{2}}\right\}}{(\cos^{-1}z-z(1-z^2)^{\frac{1}{2}})^{3/2}}\right\} \tag{B3}$$

Substituting from (3.13) into the expression for $(F-N\zeta)_1$ obtained from (5.3) and (5.4), we have to evaluate an integral of the form

$$\sum_{n=0}^{\infty}\int_{-1}^{1} x(z)\,\frac{\partial y(z)}{\partial z}\,(E-\beta Hy(z))^{\frac{1}{2}}dz. \tag{B4}$$

We cannot expand each factor in a Taylor series in $1/R$, since the last factor has a branch point when $E = \beta Hy(z)$, and we wish to integrate over z. Hence we change variables in (B4) from z to t, where z(t) is defined such that with accuracy through terms in

$1/R$, $z(t) = t + q(t)/R$ and

$$y(z(t)) = y_o(t), \tag{B5}$$

where $y_o(z)$ is obtained from (B2) by dropping the $1/R$ term and is the same as in (3.14). We find readily that to this accuracy (B4) becomes

$$\sum_{n=o}^{\infty} \int_{-1}^{1} x\left(t + \frac{q(t)}{R}\right) \frac{\partial y_o(t)}{\partial t}(E - \beta H y_o(t))^{\frac{1}{2}}\, dt. \tag{B6}$$

We obtain $x(t+q(t)/R)$ from (B3) after determining $q(t)$ from (B5) and (B2), and the integral (B6) is then readily evaluated with the methods of Section V and Appendix A. We find for the $r = 0$ correction to $(F-N\zeta)_1$

$$-\frac{3L}{105\pi} \left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{1}{(\beta H)^2} \int_o^{\infty} \frac{\partial f_o}{\partial E} E^{7/2}\, dE, \tag{B7}$$

which cancels the corresponding terms of $(F-N\zeta)_2$ and $(F-N\zeta)_+$ in (5.22) and (5.24), in agreement with Osborne's theorem. For the correction to be added to the steady part of $(F-N\zeta)_2$ we obtain

$$\frac{L}{(\beta H)^{1/3}} \left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{(\frac{3}{2})^{5/3}\, \zeta(5/3)(1 - \frac{1}{2^{2/3}})}{81\sqrt{\pi}\, \Gamma(17/6)} \int_o^{\infty} \frac{\partial f_o}{\partial E} E^{11/6}\, dE\ , \tag{B8}$$

which contributes M_{1s}, already included in (5.29)

Appendix C.

To prove (6.8) we use Poisson's sum in its usual form[31]

$$\sum_{s=1}^{\infty} f(s) + \frac{1}{2} f(o) = \sum_{n=-\infty}^{\infty} \int_{o}^{\infty} f(s)e^{2\pi ins}\, ds. \qquad (C1)$$

We now let $f(s) = g(s+\alpha)$, $0 < \alpha < 1$, and follow the method used by Dingle for $\alpha = 1/2$:

$$\sum_{s=o}^{\infty} g(s+\alpha) = \frac{1}{2} g(\alpha) + \sum_{n=-\infty}^{\infty} \int_{-\alpha}^{\infty} g(s+\alpha)e^{2\pi ins}\, ds$$

$$- \sum_{n=-\infty}^{\infty} \int_{-\alpha}^{o} g(s+\alpha)e^{2\pi ins}\, ds. \qquad (C2)$$

The general Fourier series for a function defined in $(-L,L)$ is

$$p(x) \sim \frac{1}{2L} \sum_{n=-\infty}^{\infty} e^{-\frac{\pi inx}{L}} \int_{-L}^{L} p(x')\, e^{\frac{\pi inx'}{L}}\, dx' , \qquad (C3)$$

in which the series converges to $\frac{1}{2}\left\{p(x-0) + p(x+0)\right\}$ at a point of ordinary discontinuity and to $\frac{1}{2}\left\{p(L-0) + p(-L+0)\right\}$ at $\pm L$. Hence setting $L = \frac{1}{2}$ and defining

$$p(x) = \begin{cases} g(x + \alpha - \frac{1}{2}) & \text{for } \frac{1}{2} - \alpha < x < \frac{1}{2} , \\ 0 & \text{for } -\frac{1}{2} < x < \frac{1}{2} - \alpha, \end{cases} \qquad (C4)$$

we find on substituting in (C3) and setting $x = \frac{1}{2}$

$$\frac{1}{2}g(\alpha) = \sum_{n=-\infty}^{\infty} (-1)^n \int_{\frac{1}{2}-\alpha}^{\frac{1}{2}} g(s+\alpha-\tfrac{1}{2})e^{2\pi ins}\, ds$$

$$= \sum_{n=-\infty}^{\infty} \int_{-\alpha}^{o} g(s+\alpha)e^{2\pi ins}\, ds. \qquad (C5)$$

Hence the first and third terms on the right of (C2) cancel, and we have left

$$\sum_{s=0}^{\infty} g(s+\alpha) = \sum_{n=-\infty}^{\infty} e^{-2\pi i n\alpha} \int_0^{\infty} g(s)\, e^{2\pi i n s}\, ds. \quad (C6)$$

* * * * * *

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2. E. H. Sondheimer and A. H. Wilson, Proc. Roy. Soc. (Lond.) A210, 173 (1951). This paper will be referred to in Section V as S-W.

3. R. B. Dingle, Proc. Roy. Soc. (Lond.) A211, I.500, II. 517 (1952); A212, III. 38, IV. 47 (1952).

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5. J. H. Van Vleck, Theory of Electric and Magnetic Susceptibilities, Oxford, 1932, pp. 353 ff.

6. E. Teller, Z. Physik, 67, 311 (1931).

7. M. F. M. Osborne, Phys. Rev. 88, 438 (1952).

8. M. C. Steele, Phys. Rev. 88, 451 (1952).

9. L. Landau, Z. Physik 64, 629 (1930).

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11. R. Peierls, Z. Physik 80, 763 (1933); 81, 186 (1933).

12. M. Blackman, Proc. Roy. Soc. (Lond.) A166, 1 (1938).

13. A more complete bibliography is given in the papers by Dingle.

14. J. H. van Leeuwen, Dissertation, Leiden (1919); Summary in J. Phys., Paris 2, 361 (1921).

15. Van Vleck, op. cit., Chap. IV.

16. Throughout this paper the quantity H is to be understood to be the absolute value of the magnetic field strength.

17. Since $V(r)$ has an infinite step at $r = R$, we should impose on $f(r)$ the boundary condition $f(R) = 0$. This leads in (3.5) to $(n + 3/4)$ in place of $(n + 1/2)$ when the upper limit of integration is R, although it is not clear at what point as r_2 approaches R we should start to vary from 1/2 to 3/4. This replacement does not alter the results of Section IV or the derivation of M_0 in Section V but does change the correction terms. This matter is discussed at length in Section VI, but until that section we shall use $(n + 1/2)$. Proper use of $(n + 3/4)$ would cause the curves of Fig. I to rise at a slightly lower value of x and remain slightly above the curves plotted. It would undoubtedly smooth out the low end of the moment curves in Fig. II.

18. Peirce, A Short Table of Integrals, New York, 1910, No. 187.

19. The effect of spin should be determined by Dingle's procedure (see reference 3, I). This adds to the steady moment the usual spin paramagnetism and changes the phase of the oscillatory terms.

20. The tail is clearly defined only if we use approximate methods, such as the WKB procedure, to determine the energy eigenvalues. In an exact solution all eigenvalues would depend on r_0, but the departure from the free electron eigenvalues would be appreciable only for states with $r_0 \gtrsim R$.

21. When we obtain M from (5.3) we should have no terms involving $[\partial\delta(n,H,E)]/\partial H$ or $\partial\Delta r_{on}/\partial H$ and in fact do not, for although both $\delta(n,H,E)$ and Δr_{on} depend on H, $(E-\varepsilon)^{\frac{1}{2}}$ vanishes at $r_o=\delta$ and $\partial\varepsilon/\partial r_o$ vanishes at $r_o=R - \Delta r_{on}$, so that the integrand is zero at each limit of integration.

22. E. T. Whittaker and G. N. Watson, A Course of Modern Analysis, 4th ed. Cambridge, 1952, p. 337.

23. Whittaker & Watson, op. cit. $M_{k,m}(z)$ is incorrectly given in terms of $W_{k,m}(z)$ and $W_{-k,m}(-z)$ in Ex. 2 of §16.41, p. 346. The expression should be corrected by replacing $e^{k\pi i}$ by $e^{-k\pi i}$ in each term. The asymptotic expansion of $W_{k,m}(z)$ is given on p. 343.

24. This theorem, one form of which was previously suggested by Dingle (Ref. 3, III), has proved to be true to the accuracy used in every problem in which it has been tested, including our exact solution of the Darwin problem (Section VII). No one has as yet given a general proof; Osborne's proof is valid for fairly general potentials but requires the use of the WKB approximation, which is known to be accurate only asymptotically as either $(\hbar^2/m) \to 0$, or as the quantum number n becomes large (J. L. Dunham, Phys. Rev. 41, 713 (1932)). Since this is in this sense a semiclassical approximation, it is not impossible that its use obscures a purely quantum effect

not shown by Darwin's model.

25. The magnitude of the M_1 correction was incorrectly given in the abstract of an earlier report on this work. Moreover, at the time of that report the work of Section VI had not been done. (Bull. Amer. Phys. Soc. 28, no. 1 WA8.)

26. Several of our small oscillatory terms correspond to terms found by Osborne. Thus the second term in his $M_{1,0,0}$ is of the same form as the oscillatory part of our M_1, and his $M_{1,1,0}$ is like the oscillatory part of M_+, or M_2 and arises from the energy surface near states with positive s.

27. L. I. Schiff, Quantum Mechanics, McGraw-Hill, New York, 1949, p. 186.

28. Whittaker and Watson, op. cit., p. 244.

29. See Reference 8, Appendix. Steele's integrals are very similar to ours. Thus his I_{11} is apart from a constant the imaginary part of our $V_{0,-\frac{1}{2}}(\omega/2)$. His I_{12} is proportional to $\mathrm{Im}\, V_{1,-\frac{1}{2}}(\omega/2)$, and his $I_{21}+I_{22}$ to

$$\mathrm{Im}\left\{\int_{-1}^{1} dz\, V_{\frac{1}{2},-\frac{1}{2}}\left(\frac{\omega}{2g(z)}\right)\right\}$$

30. Proceedings of the Section of Sciences, Nederlandsche Akademie Van Wetenschappen 51, 650 (1948).

31. Reference 3, I (Appendix). The conditions for the validity of the formula and the sense in which the convergence of the series is to be understood are obtained from Titchmarsh, Introduction to the Theory of Fourier Integrals, Oxford, 1932, p. 60.